



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:11 pm BST

PDB ID : 4MLA
Title : Structure of maize cytokinin oxidase/dehydrogenase 2 (ZmCKO2)
Authors : Morera, S.; Kopečný, D.; Briozzo, P.; Koncitikova, R.
Deposited on : 2013-09-06
Resolution : 2.04 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

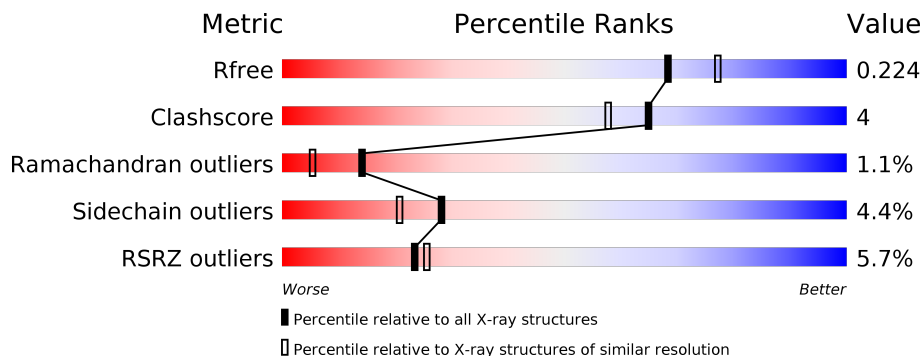
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	501	 6% 85% 9% • 5%
1	B	501	 5% 80% 11% • 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8004 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.

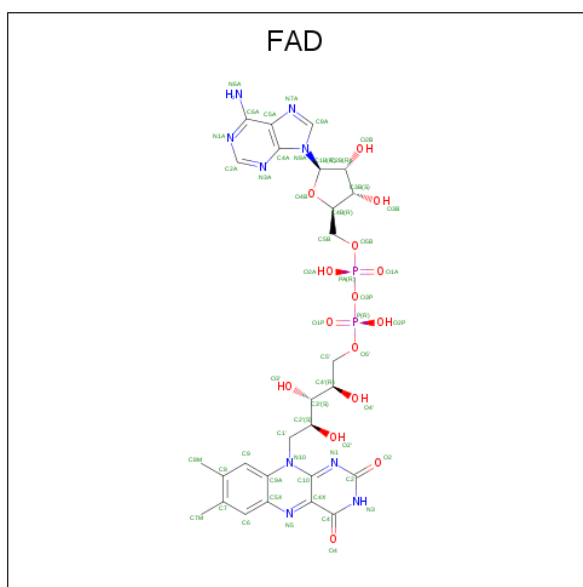
- Molecule 1 is a protein called Cytokinin oxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	477	3760	2392	662	692	14	0	0	0
1	B	460	3619	2303	634	668	14	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

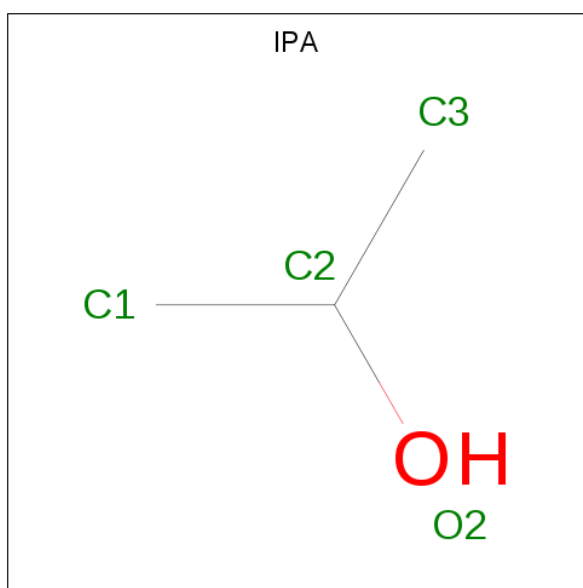
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ALA	-	EXPRESSION TAG	UNP Q709Q5
A	17	GLY	-	EXPRESSION TAG	UNP Q709Q5
A	18	HIS	-	EXPRESSION TAG	UNP Q709Q5
A	19	MET	-	EXPRESSION TAG	UNP Q709Q5
B	16	ALA	-	EXPRESSION TAG	UNP Q709Q5
B	17	GLY	-	EXPRESSION TAG	UNP Q709Q5
B	18	HIS	-	EXPRESSION TAG	UNP Q709Q5
B	19	MET	-	EXPRESSION TAG	UNP Q709Q5

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



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

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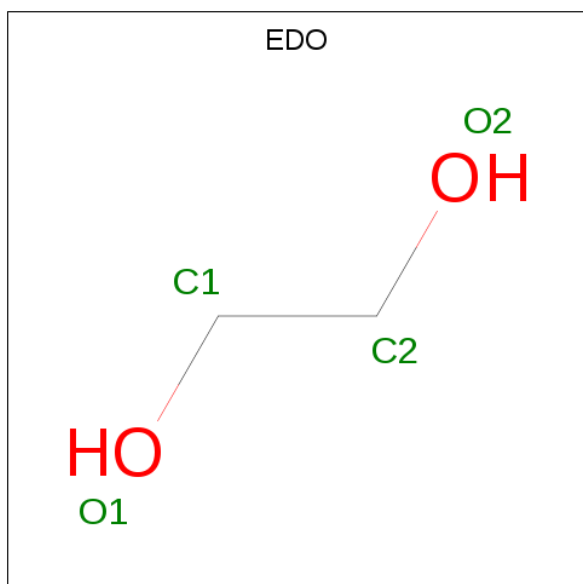
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



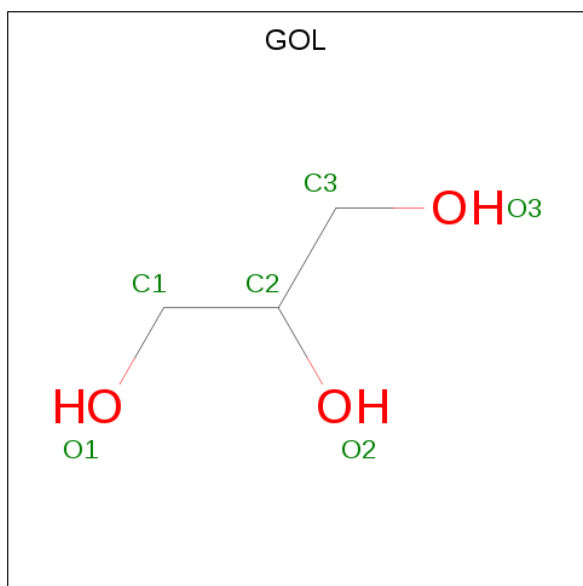
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

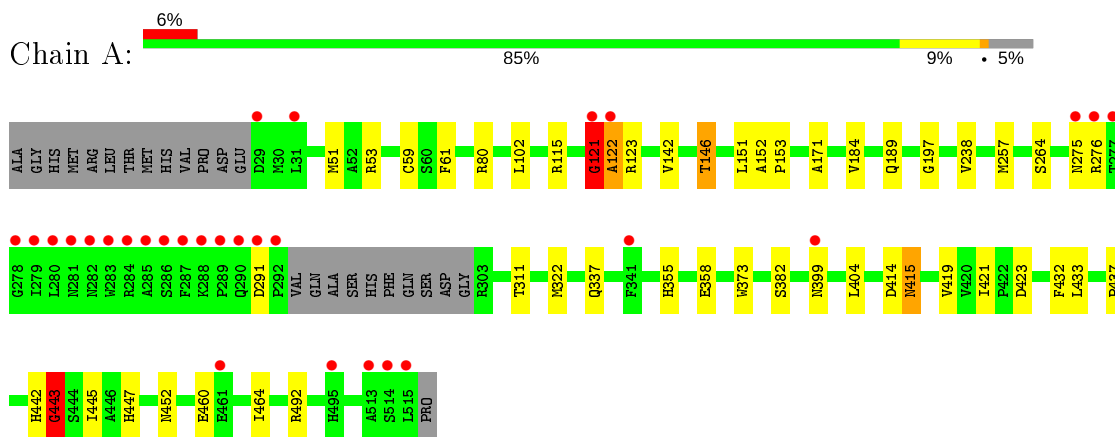
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	183	Total	O	0	0
			183	183		
6	B	178	Total	O	0	0
			178	178		

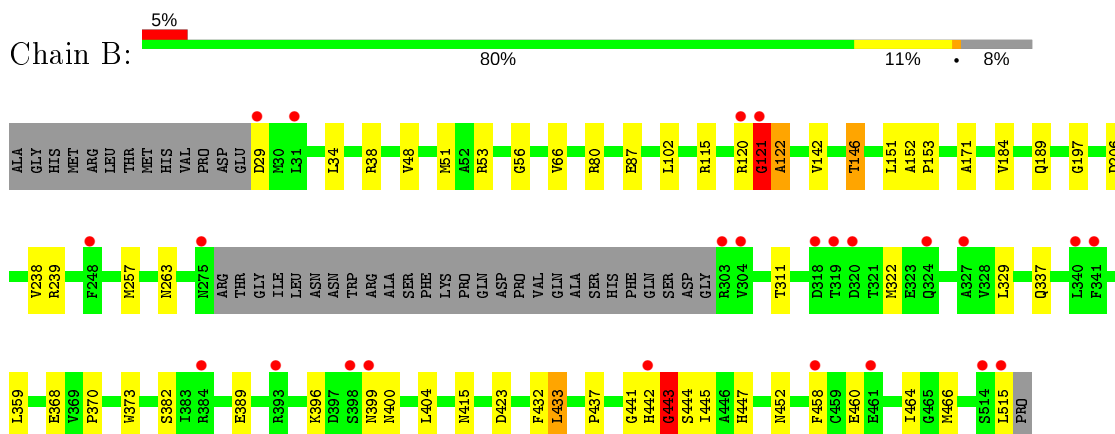
3 Residue-property plots [i](#)

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

- Molecule 1: Cytokinin oxidase 2



- Molecule 1: Cytokinin oxidase 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	75.72Å 181.89Å 196.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.56 – 2.04 47.86 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.0 (23.56-2.04) 99.2 (47.86-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.05Å)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.193 , 0.222 0.198 , 0.224	Depositor DCC
R_{free} test set	4289 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtrriage
Anisotropy	0.364	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8004	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to $7.1077e-05$. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, IPA, EDO, 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	0.51	0/3853	0.68	2/5229 (0.0%)
1	B	0.49	0/3707	0.70	4/5030 (0.1%)
All	All	0.50	0/7560	0.69	6/10259 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	GLY	C-N-CA	6.11	136.98	121.70
1	B	121	GLY	C-N-CA	5.82	136.25	121.70
1	B	443	GLY	C-N-CA	5.80	136.21	121.70
1	A	121	GLY	C-N-CA	5.26	134.86	121.70
1	B	87	GLU	N-CA-C	5.15	124.92	111.00
1	B	87	GLU	C-N-CA	5.07	132.95	122.30

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	3760	0	3687	30	0
1	B	3619	0	3549	31	0
2	A	53	0	29	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	29	1	0
3	A	68	0	134	4	0
3	B	48	0	95	9	0
4	A	20	0	30	3	0
4	B	4	0	6	0	0
5	A	6	0	8	2	0
5	B	12	0	16	0	0
6	A	183	0	0	1	0
6	B	178	0	0	1	0
All	All	8004	0	7583	63	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 4.

All (63) 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:121:GLY:HA3	1:A:122:ALA:CB	2.00	0.91
1:B:121:GLY:HA3	1:B:122:ALA:CB	2.08	0.84
1:A:432:PHE:HB3	5:A:609:GOL:H11	1.61	0.82
1:A:121:GLY:HA3	1:A:122:ALA:HB2	1.64	0.79
1:B:121:GLY:HA3	1:B:122:ALA:HB2	1.74	0.68
1:A:146:THR:HG23	1:A:151:LEU:O	1.94	0.68
1:B:466:MET:H	3:B:607:IPA:H13	1.59	0.67
1:A:189:GLN:HE21	3:A:603:IPA:H32	1.60	0.67
1:B:146:THR:HG23	1:B:151:LEU:O	1.96	0.66
1:A:121:GLY:HA3	1:A:122:ALA:HB3	1.78	0.65
1:A:189:GLN:HG2	3:A:603:IPA:H13	1.80	0.64
1:B:189:GLN:HE21	3:B:611:IPA:H2	1.63	0.62
1:B:51:MET:HE1	1:B:115:ARG:HG3	1.82	0.61
1:A:414:ASP:HA	4:A:605:EDO:H22	1.82	0.61
1:B:121:GLY:HA3	1:B:122:ALA:HB3	1.83	0.61
1:A:452:ASN:OD1	5:A:609:GOL:H2	2.02	0.60
1:A:146:THR:CG2	1:A:152:ALA:HA	2.32	0.59
1:A:146:THR:HG21	1:A:153:PRO:HD3	1.87	0.57
1:B:437:PRO:HD2	1:B:443:GLY:O	2.04	0.57
1:B:452:ASN:OD1	3:B:613:IPA:H13	2.05	0.56
1:B:415:ASN:HA	3:B:612:IPA:H32	1.87	0.56
1:A:437:PRO:HD2	1:A:443:GLY:O	2.06	0.56
1:B:146:THR:CG2	1:B:152:ALA:HA	2.35	0.56
1:B:238:VAL:HG13	1:B:311:THR:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:THR:HG21	1:B:153:PRO:HD3	1.89	0.53
1:A:51:MET:HE1	1:A:115:ARG:HG3	1.90	0.53
1:B:466:MET:N	3:B:607:IPA:H13	2.23	0.53
1:B:404:LEU:HD13	1:B:433:LEU:HD22	1.91	0.52
1:B:432:PHE:HB3	3:B:613:IPA:H12	1.90	0.52
1:A:355:HIS:HD2	1:A:358:GLU:OE1	1.93	0.52
1:A:146:THR:HG23	1:A:152:ALA:HA	1.93	0.51
1:B:382:SER:HB3	1:B:464:ILE:HG13	1.93	0.51
1:A:404:LEU:HD13	1:A:433:LEU:HD22	1.93	0.50
1:B:53:ARG:HD3	6:B:726:HOH:O	2.12	0.50
1:B:460:GLU:HA	3:B:607:IPA:H2	1.93	0.50
1:B:146:THR:HG23	1:B:152:ALA:HA	1.94	0.48
1:A:142:VAL:O	1:A:146:THR:HB	2.13	0.48
1:B:433:LEU:HD11	3:B:609:IPA:H2	1.95	0.48
1:A:382:SER:HB3	1:A:464:ILE:HG13	1.96	0.47
1:A:121:GLY:CA	1:A:122:ALA:CB	2.83	0.47
2:A:601:FAD:C4	3:A:610:IPA:H32	2.46	0.46
1:A:460:GLU:HA	3:A:614:IPA:H2	1.98	0.45
2:B:602:FAD:C4	3:B:609:IPA:H32	2.46	0.45
1:A:80:ARG:HG3	1:A:197:GLY:HA3	1.97	0.45
1:B:441:GLY:O	1:B:444:SER:HB3	2.17	0.45
1:A:415:ASN:H	4:A:605:EDO:H21	1.81	0.45
1:A:442:HIS:O	1:A:447:HIS:CD2	2.70	0.45
1:B:442:HIS:O	1:B:447:HIS:HD2	2.00	0.44
1:B:442:HIS:O	1:B:447:HIS:CD2	2.71	0.44
1:B:146:THR:HG21	1:B:152:ALA:HA	1.99	0.43
1:B:48:VAL:HG12	1:B:66:VAL:HG23	2.00	0.43
1:A:419:VAL:HG12	1:A:421:ILE:HG23	2.00	0.43
1:A:238:VAL:HG13	1:A:311:THR:HB	2.00	0.42
1:A:415:ASN:H	4:A:605:EDO:C2	2.32	0.42
1:B:80:ARG:HG3	1:B:197:GLY:HA3	2.01	0.42
1:A:146:THR:HG21	1:A:152:ALA:HA	2.00	0.42
1:B:102:LEU:HD13	1:B:373:TRP:HB2	2.03	0.41
1:A:102:LEU:HD13	1:A:373:TRP:HB2	2.02	0.41
1:B:56:GLY:O	1:B:370:PRO:HA	2.20	0.41
1:A:59:CYS:HB3	1:A:61:PHE:CE2	2.56	0.40
1:B:389:GLU:HG2	1:B:458:PHE:CD1	2.56	0.40
1:B:142:VAL:O	1:B:146:THR:HB	2.21	0.40
1:A:53:ARG:HD3	6:A:706:HOH:O	2.20	0.40

There are no symmetry-related clashes.

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	473/501 (94%)	452 (96%)	15 (3%)	6 (1%)	12	4
1	B	456/501 (91%)	433 (95%)	19 (4%)	4 (1%)	17	8
All	All	929/1002 (93%)	885 (95%)	34 (4%)	10 (1%)	14	5

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ALA
1	B	122	ALA
1	A	121	GLY
1	A	171	ALA
1	B	121	GLY
1	A	123	ARG
1	A	264	SER
1	B	171	ALA
1	A	443	GLY
1	B	443	GLY

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	405/425 (95%)	392 (97%)	13 (3%)	39	32
1	B	390/425 (92%)	368 (94%)	22 (6%)	21	12
All	All	795/850 (94%)	760 (96%)	35 (4%)	28	21

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	THR
1	A	184	VAL
1	A	257	MET
1	A	275	ASN
1	A	276	ARG
1	A	291	ASP
1	A	322	MET
1	A	337	GLN
1	A	399	ASN
1	A	415	ASN
1	A	423	ASP
1	A	445	ILE
1	A	492	ARG
1	B	29	ASP
1	B	34	LEU
1	B	38	ARG
1	B	120	ARG
1	B	146	THR
1	B	184	VAL
1	B	206	ASP
1	B	239	ARG
1	B	257	MET
1	B	263	ASN
1	B	322	MET
1	B	329	LEU
1	B	337	GLN
1	B	359	LEU
1	B	368	GLU
1	B	396	LYS
1	B	399	ASN
1	B	400	ASN
1	B	423	ASP
1	B	433	LEU
1	B	445	ILE
1	B	515	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	188	ASN

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Mol	Chain	Res	Type
1	A	189	GLN
1	A	281	ASN
1	A	282	ASN
1	A	337	GLN
1	A	355	HIS
1	A	415	ASN
1	A	447	HIS
1	A	468	GLN
1	A	476	GLN
1	B	68	HIS
1	B	188	ASN
1	B	189	GLN
1	B	447	HIS
1	B	468	GLN
1	B	476	GLN
1	B	478	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](#)

40 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
3	IPA	B	608	-	3,3,3	0.59	0	3,3,3	0.53	0
3	IPA	A	611	-	3,3,3	0.82	0	3,3,3	0.66	0
3	IPA	A	618	-	3,3,3	0.65	0	3,3,3	0.50	0
3	IPA	B	612	-	3,3,3	0.58	0	3,3,3	0.86	0
4	EDO	A	624	-	3,3,3	0.61	0	2,2,2	0.49	0
3	IPA	A	606	-	3,3,3	0.58	0	3,3,3	0.83	0
5	GOL	A	609	-	5,5,5	0.06	0	5,5,5	0.21	0
3	IPA	A	613	-	3,3,3	0.70	0	3,3,3	0.56	0
5	GOL	B	615	-	5,5,5	0.06	0	5,5,5	0.13	0
3	IPA	A	620	-	3,3,3	0.44	0	3,3,3	0.73	0
3	IPA	A	612	-	3,3,3	0.70	0	3,3,3	0.82	0
3	IPA	B	610	-	3,3,3	0.65	0	3,3,3	0.60	0
3	IPA	A	604	-	3,3,3	0.56	0	3,3,3	0.51	0
3	IPA	A	616	-	3,3,3	0.60	0	3,3,3	0.58	0
3	IPA	B	604	-	3,3,3	0.65	0	3,3,3	0.60	0
2	FAD	A	601	1	51,58,58	1.53	5 (9%)	60,89,89	2.31	11 (18%)
3	IPA	A	622	-	3,3,3	0.77	0	3,3,3	0.54	0
3	IPA	B	616	-	3,3,3	0.66	0	3,3,3	0.54	0
4	EDO	A	605	-	3,3,3	0.69	0	2,2,2	0.08	0
3	IPA	B	601	-	3,3,3	1.13	0	3,3,3	0.94	0
4	EDO	A	607	-	3,3,3	0.62	0	2,2,2	0.38	0
3	IPA	A	610	-	3,3,3	0.46	0	3,3,3	0.62	0
3	IPA	A	602	-	3,3,3	0.86	0	3,3,3	0.58	0
3	IPA	B	607	-	3,3,3	0.65	0	3,3,3	0.31	0
3	IPA	A	615	-	3,3,3	0.76	0	3,3,3	0.58	0
3	IPA	A	621	-	3,3,3	0.68	0	3,3,3	0.72	0
2	FAD	B	602	1	51,58,58	1.42	5 (9%)	60,89,89	2.32	11 (18%)
3	IPA	B	606	-	3,3,3	0.66	0	3,3,3	0.56	0
4	EDO	A	623	-	3,3,3	0.74	0	2,2,2	0.29	0
4	EDO	B	605	-	3,3,3	0.69	0	2,2,2	0.31	0
5	GOL	B	603	-	5,5,5	0.16	0	5,5,5	0.51	0
3	IPA	A	617	-	3,3,3	0.47	0	3,3,3	0.60	0
3	IPA	A	619	-	3,3,3	0.74	0	3,3,3	0.51	0
3	IPA	B	614	-	3,3,3	0.78	0	3,3,3	0.63	0
3	IPA	A	603	-	3,3,3	0.44	0	3,3,3	0.52	0
3	IPA	B	611	-	3,3,3	0.66	0	3,3,3	0.61	0
4	EDO	A	608	-	3,3,3	0.67	0	2,2,2	0.31	0
3	IPA	B	609	-	3,3,3	0.41	0	3,3,3	0.57	0
3	IPA	A	614	-	3,3,3	0.84	0	3,3,3	0.42	0
3	IPA	B	613	-	3,3,3	0.78	0	3,3,3	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	605	-	-	1/1/1/1	-
2	FAD	A	601	1	-	7/30/50/50	0/6/6/6
2	FAD	B	602	1	-	7/30/50/50	0/6/6/6
4	EDO	A	623	-	-	1/1/1/1	-
4	EDO	A	605	-	-	0/1/1/1	-
4	EDO	A	624	-	-	1/1/1/1	-
5	GOL	B	603	-	-	1/4/4/4	-
4	EDO	A	607	-	-	0/1/1/1	-
5	GOL	B	615	-	-	0/4/4/4	-
4	EDO	A	608	-	-	0/1/1/1	-
5	GOL	A	609	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C4X-C10	7.38	1.46	1.38
2	B	602	FAD	C4X-C10	6.93	1.45	1.38
2	A	601	FAD	C4-C4X	4.10	1.48	1.41
2	B	602	FAD	C4-N3	3.34	1.38	1.33
2	A	601	FAD	C9A-N10	3.32	1.43	1.38
2	B	602	FAD	C9A-N10	3.25	1.42	1.38
2	A	601	FAD	C4-N3	3.18	1.38	1.33
2	A	601	FAD	C5X-N5	3.16	1.40	1.35
2	B	602	FAD	C4-C4X	3.06	1.46	1.41
2	B	602	FAD	C5X-N5	2.85	1.40	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	FAD	C4-N3-C2	12.72	125.88	115.14
2	A	601	FAD	C4-N3-C2	12.59	125.78	115.14
2	A	601	FAD	C4X-C4-N3	-6.68	114.29	123.43
2	B	602	FAD	C4X-C4-N3	-6.46	114.60	123.43
2	B	602	FAD	C10-C4X-N5	4.40	124.30	121.26
2	A	601	FAD	C10-C4X-N5	4.18	124.15	121.26
2	B	602	FAD	C4-C4X-C10	-3.86	117.40	119.95
2	A	601	FAD	C4-C4X-C10	-3.74	117.48	119.95
2	B	602	FAD	C4'-C3'-C2'	3.66	120.97	113.36
2	B	602	FAD	C4X-C10-N10	-3.17	117.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C4X-C10-N10	-3.17	117.04	120.30
2	A	601	FAD	O5'-P-O1P	3.08	121.10	109.07
2	A	601	FAD	C5'-C4'-C3'	3.07	118.13	112.20
2	A	601	FAD	O5'-C5'-C4'	2.96	117.27	109.36
2	A	601	FAD	C4'-C3'-C2'	2.89	119.38	113.36
2	B	602	FAD	O5'-P-O1P	2.87	120.27	109.07
2	B	602	FAD	C5'-C4'-C3'	2.86	117.72	112.20
2	B	602	FAD	O5'-C5'-C4'	2.84	116.95	109.36
2	A	601	FAD	O2P-P-O5'	-2.72	95.12	107.75
2	B	602	FAD	O2P-P-O5'	-2.68	95.29	107.75
2	A	601	FAD	C5A-C6A-N6A	2.38	123.97	120.35
2	B	602	FAD	C5A-C6A-N6A	2.30	123.85	120.35

There are no chirality outliers.

All (20) torsion outliers are listed below:

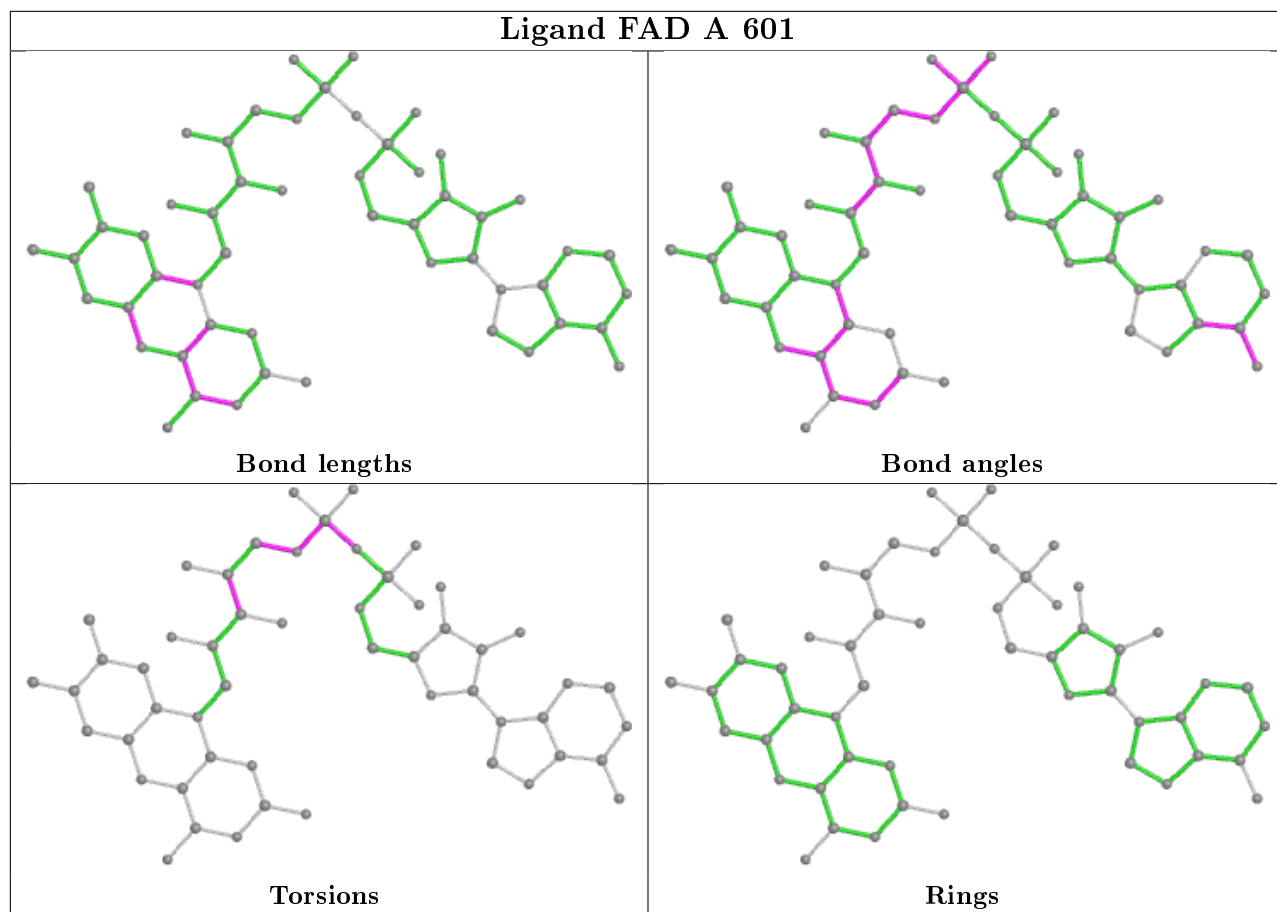
Mol	Chain	Res	Type	Atoms
5	A	609	GOL	O1-C1-C2-C3
2	B	602	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	O3'-C3'-C4'-C5'
2	B	602	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	B	602	FAD	O3'-C3'-C4'-O4'
5	A	609	GOL	O1-C1-C2-O2
2	A	601	FAD	C4'-C5'-O5'-P
2	B	602	FAD	C4'-C5'-O5'-P
4	A	624	EDO	O1-C1-C2-O2
4	A	623	EDO	O1-C1-C2-O2
2	A	601	FAD	PA-O3P-P-O1P
2	B	602	FAD	PA-O3P-P-O1P
2	A	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	PA-O3P-P-O2P
2	B	602	FAD	PA-O3P-P-O2P
4	B	605	EDO	O1-C1-C2-O2
2	A	601	FAD	C5'-O5'-P-O1P
2	B	602	FAD	C5'-O5'-P-O1P
5	B	603	GOL	O2-C2-C3-O3

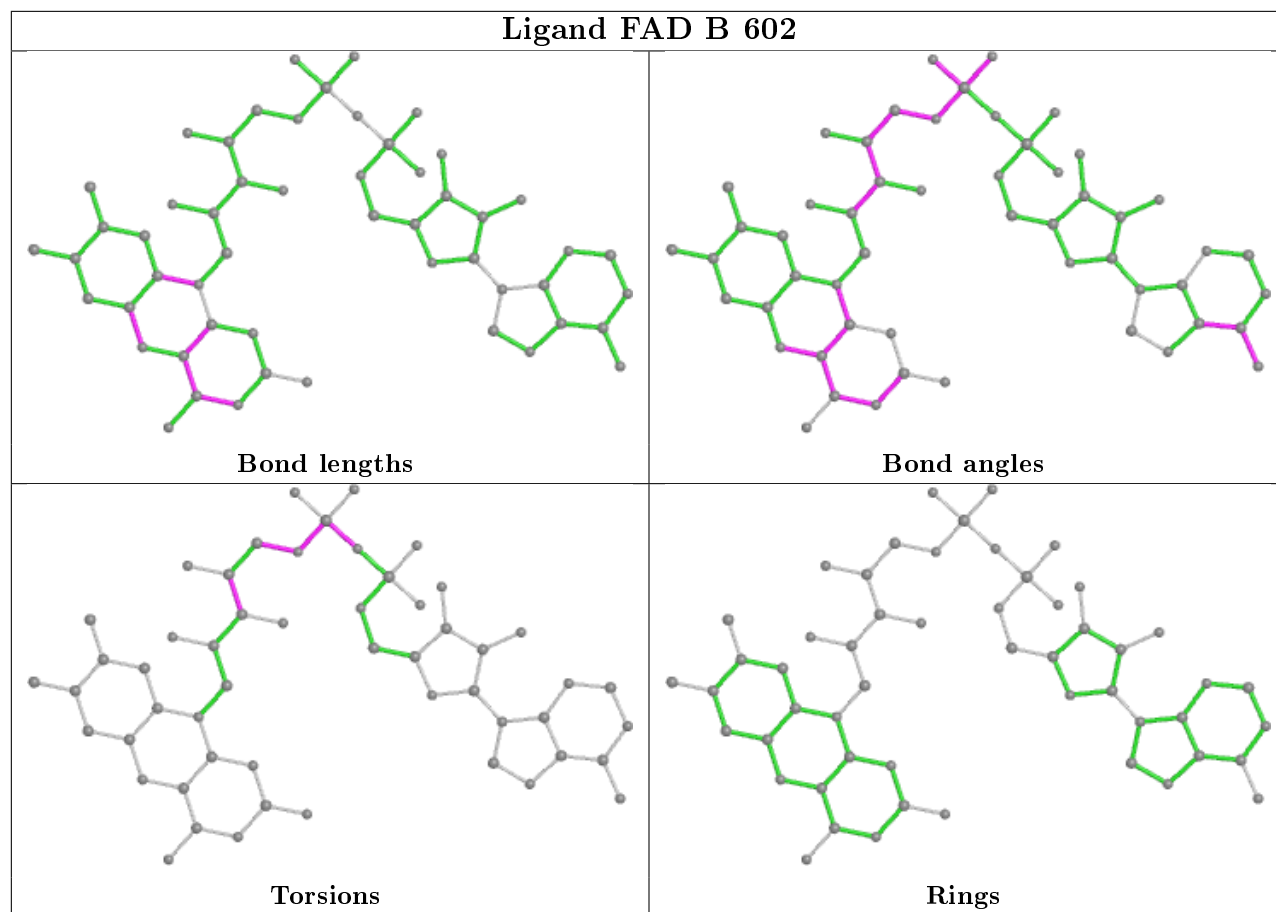
There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	612	IPA	1	0
5	A	609	GOL	2	0
2	A	601	FAD	1	0
4	A	605	EDO	3	0
3	A	610	IPA	1	0
3	B	607	IPA	3	0
2	B	602	FAD	1	0
3	A	603	IPA	2	0
3	B	611	IPA	1	0
3	B	609	IPA	2	0
3	A	614	IPA	1	0
3	B	613	IPA	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.





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	477/501 (95%)	-0.01	29 (6%) 21 22	25, 37, 78, 116	0
1	B	460/501 (91%)	0.03	24 (5%) 27 29	26, 40, 73, 106	0
All	All	937/1002 (93%)	0.01	53 (5%) 23 25	25, 39, 75, 116	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	ASN	8.0
1	A	285	ALA	7.4
1	A	291	ASP	7.1
1	A	279	ILE	6.6
1	A	283	TRP	6.4
1	A	289	PRO	6.1
1	A	286	SER	6.0
1	A	277	THR	5.7
1	B	514	SER	5.3
1	B	341	PHE	5.3
1	A	290	GLN	5.2
1	A	284	ARG	5.0
1	A	399	ASN	5.0
1	A	287	PHE	4.6
1	A	280	LEU	4.5
1	A	292	PRO	4.5
1	A	282	ASN	4.3
1	B	399	ASN	4.3
1	A	513	ALA	4.2
1	A	276	ARG	4.1
1	A	288	LYS	4.0
1	A	278	GLY	4.0
1	B	461	GLU	3.6
1	B	515	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	320	ASP	3.4
1	A	514	SER	3.4
1	B	324	GLN	3.3
1	A	341	PHE	3.1
1	A	31	LEU	3.0
1	B	340	LEU	2.9
1	A	461	GLU	2.9
1	A	121	GLY	2.8
1	B	31	LEU	2.8
1	B	248	PHE	2.6
1	B	442	HIS	2.6
1	B	121	GLY	2.5
1	A	495	HIS	2.5
1	B	327	ALA	2.4
1	B	303	ARG	2.4
1	B	318	ASP	2.4
1	B	458	PHE	2.4
1	B	319	THR	2.4
1	B	275	ASN	2.3
1	B	393	ARG	2.3
1	A	122	ALA	2.3
1	B	398	SER	2.3
1	A	29	ASP	2.2
1	B	384	ARG	2.2
1	B	29	ASP	2.2
1	B	304	VAL	2.2
1	A	275	ASN	2.0
1	A	515	LEU	2.0
1	B	120	ARG	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.

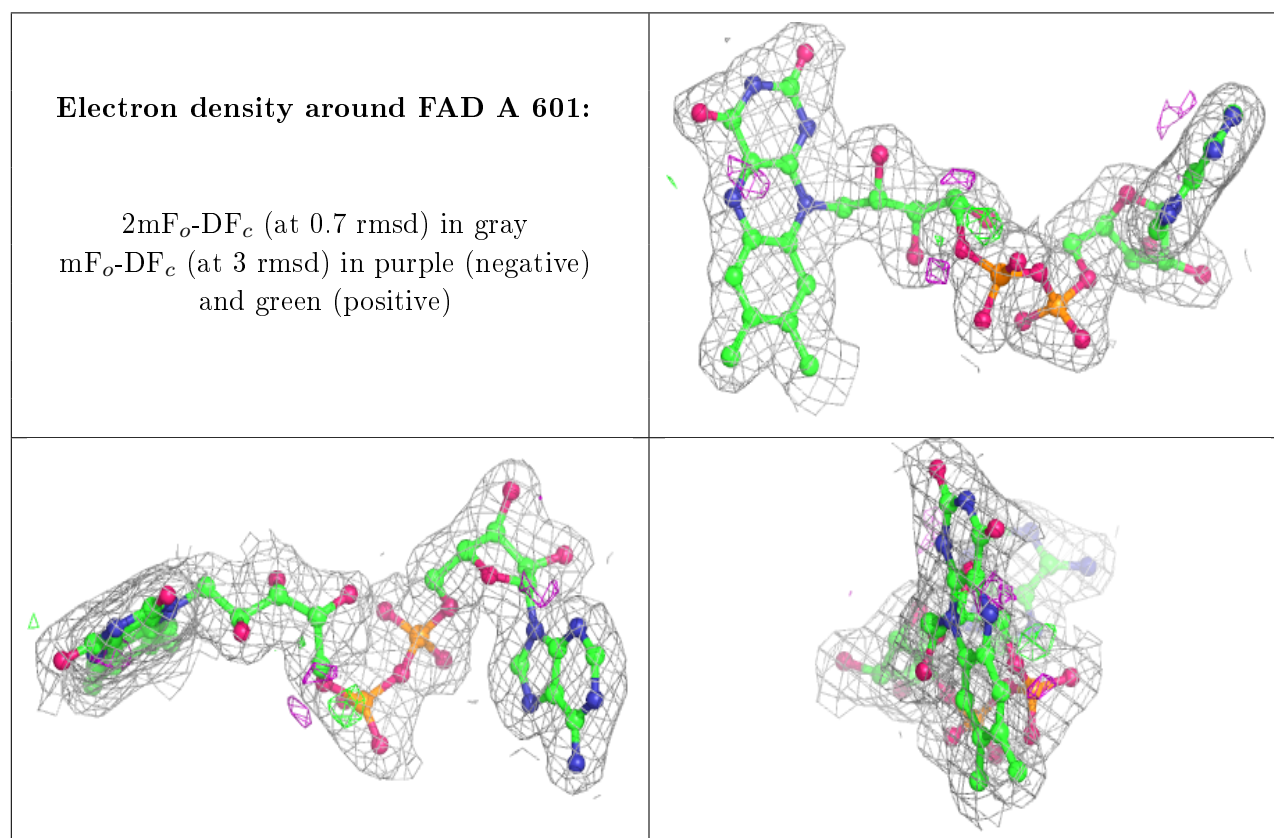
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	624	4/4	0.60	0.20	58,59,63,63	0
4	EDO	A	623	4/4	0.64	0.40	60,61,61,62	0
4	EDO	A	605	4/4	0.66	0.35	59,61,63,64	0
3	IPA	B	608	4/4	0.72	0.17	79,80,81,81	0
3	IPA	A	619	4/4	0.73	0.20	71,71,72,73	0
3	IPA	B	607	4/4	0.75	0.23	48,53,53,57	0
3	IPA	A	615	4/4	0.78	0.28	65,65,66,67	0
5	GOL	B	603	6/6	0.80	0.26	59,62,64,65	0
4	EDO	A	608	4/4	0.80	0.21	61,62,62,63	0
4	EDO	A	607	4/4	0.84	0.26	62,65,65,66	0
3	IPA	A	622	4/4	0.84	0.21	53,56,57,58	0
3	IPA	B	606	4/4	0.85	0.23	63,65,66,67	0
3	IPA	A	621	4/4	0.86	0.25	61,61,61,62	0
3	IPA	A	614	4/4	0.86	0.15	44,45,47,49	0
5	GOL	B	615	6/6	0.87	0.19	70,72,74,74	0
3	IPA	A	612	4/4	0.87	0.31	43,44,45,50	0
3	IPA	A	604	4/4	0.87	0.25	48,49,50,53	0
3	IPA	B	613	4/4	0.87	0.14	48,51,52,53	0
4	EDO	B	605	4/4	0.88	0.17	61,61,61,62	0
3	IPA	B	614	4/4	0.89	0.17	56,58,58,59	0
3	IPA	A	620	4/4	0.91	0.23	57,57,57,60	0
3	IPA	A	606	4/4	0.92	0.21	48,50,50,54	0
3	IPA	B	616	4/4	0.92	0.37	68,68,69,69	0
3	IPA	A	617	4/4	0.92	0.15	47,51,53,55	0
3	IPA	B	604	4/4	0.92	0.32	57,60,60,61	0
3	IPA	A	603	4/4	0.93	0.27	63,64,65,66	0
3	IPA	B	612	4/4	0.93	0.19	42,42,46,49	0
3	IPA	A	613	4/4	0.93	0.21	59,60,61,63	0
3	IPA	A	616	4/4	0.94	0.34	61,61,61,62	0
5	GOL	A	609	6/6	0.94	0.18	61,62,63,65	0
3	IPA	B	611	4/4	0.95	0.18	45,49,49,50	0
3	IPA	B	609	4/4	0.95	0.30	54,58,59,60	0
3	IPA	B	610	4/4	0.96	0.18	51,55,56,57	0
3	IPA	A	618	4/4	0.96	0.10	50,50,51,54	0
3	IPA	A	602	4/4	0.97	0.18	38,38,40,43	0
3	IPA	A	610	4/4	0.97	0.25	54,56,57,58	0
3	IPA	B	601	4/4	0.97	0.22	31,34,34,39	0

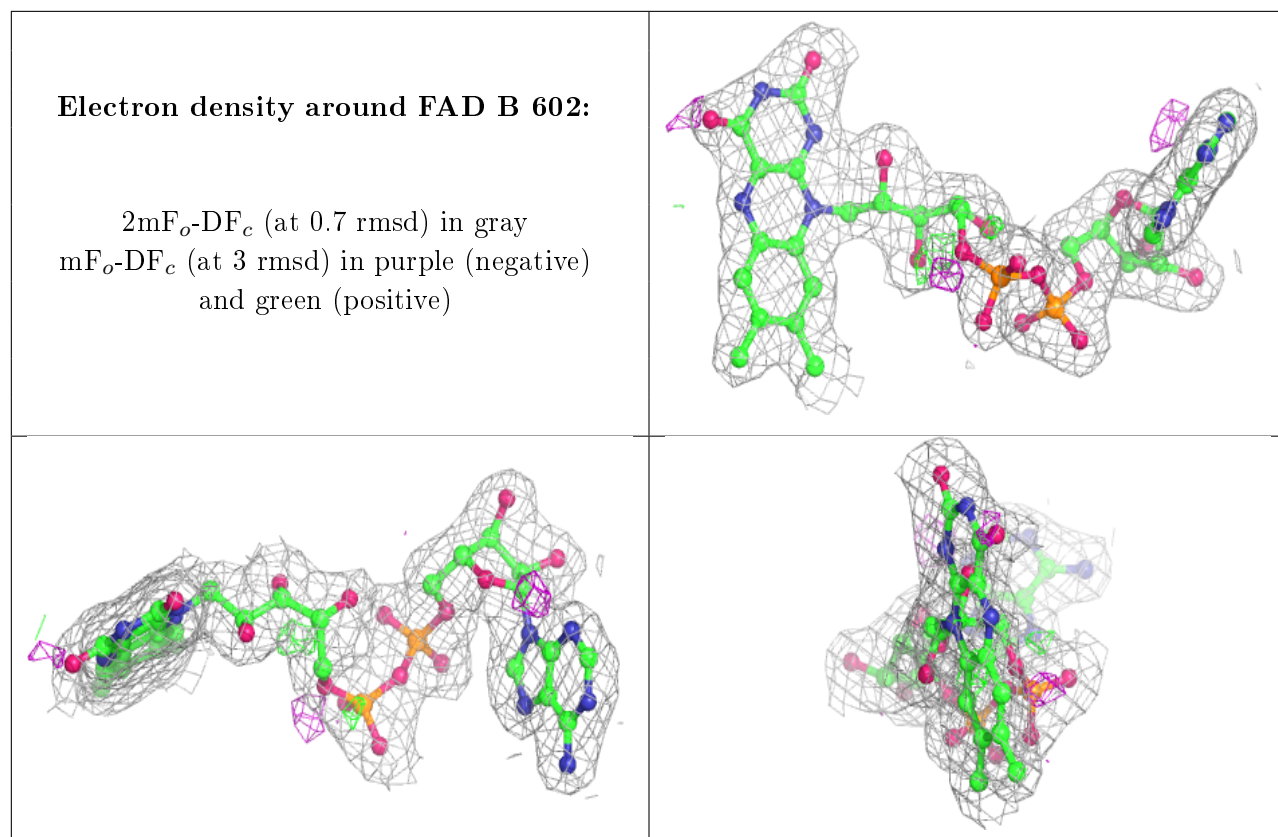
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	IPA	A	611	4/4	0.97	0.22	35,37,37,40	0
2	FAD	A	601	53/53	0.97	0.11	23,30,33,37	0
2	FAD	B	602	53/53	0.97	0.13	21,30,37,39	0

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.