



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:05 AM UTC

PDB ID : 3WGT / pdb_00003wgt
Title : Crystal structure of D-amino acid oxidase mutant
Authors : Yasukawa, K.; Nakano, S.; Asano, Y.
Deposited on : 2013-08-09
Resolution : 1.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

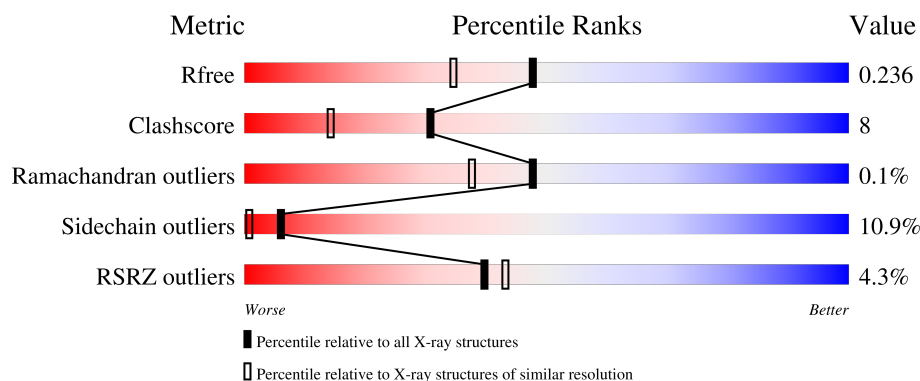
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	347	 5% 79% 17% ...
1	B	347	 3% 78% 16% ...

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
4	SO4	A	404	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 5753 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.

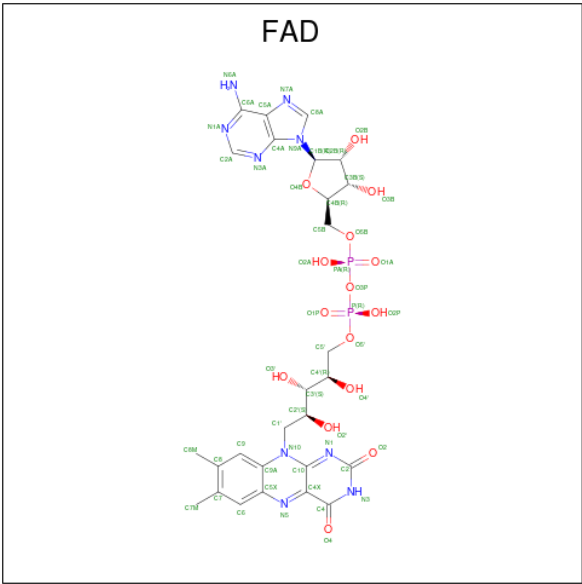
- Molecule 1 is a protein called D-amino-acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2724	1752	472	491	9			
1	B	339	Total	C	N	O	S	0	0	0
			2709	1742	470	488	9			

There are 4 discrepancies between the modelled and reference sequences:

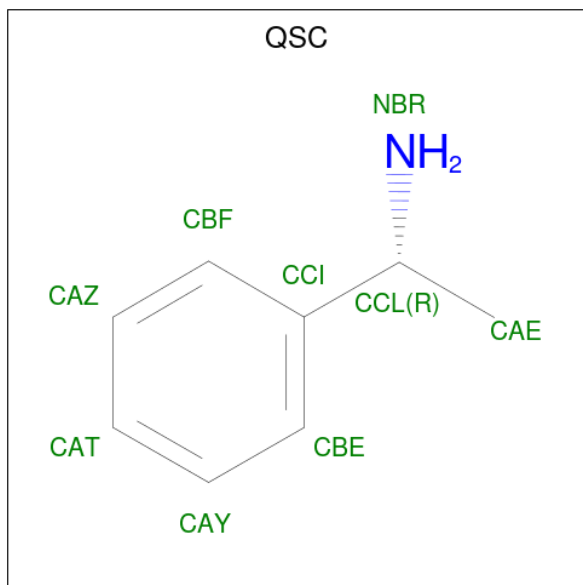
Chain	Residue	Modelled	Actual	Comment	Reference
A	228	LEU	TYR	engineered mutation	UNP P00371
A	283	GLY	ARG	engineered mutation	UNP P00371
B	228	LEU	TYR	engineered mutation	UNP P00371
B	283	GLY	ARG	engineered mutation	UNP P00371

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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 (1R)-1-phenylethylamine (CCD ID: QSC) (formula: C₈H₁₁N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	8	1		
3	B	1	Total	C	N	0	0
			9	8	1		

- Molecule 4 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

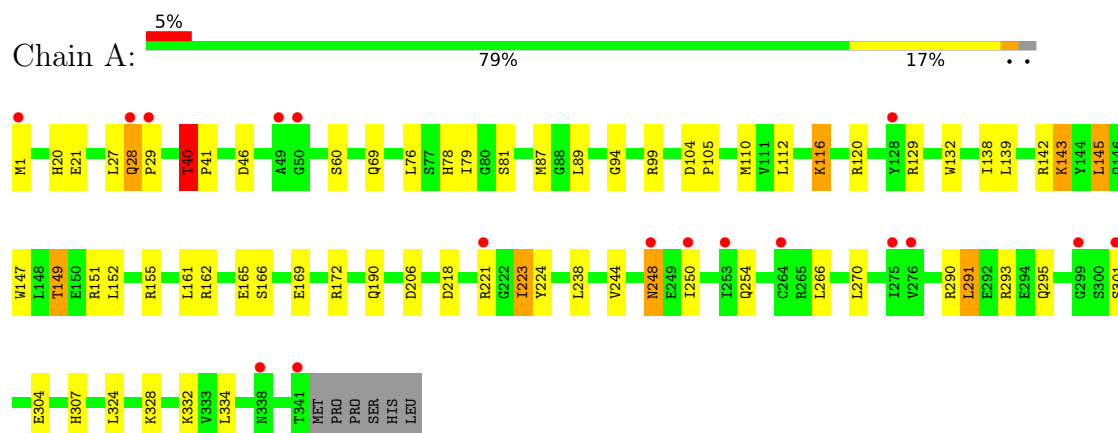
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	94	Total	O	0	0
			94	94		
5	B	82	Total	O	0	0
			82	82		

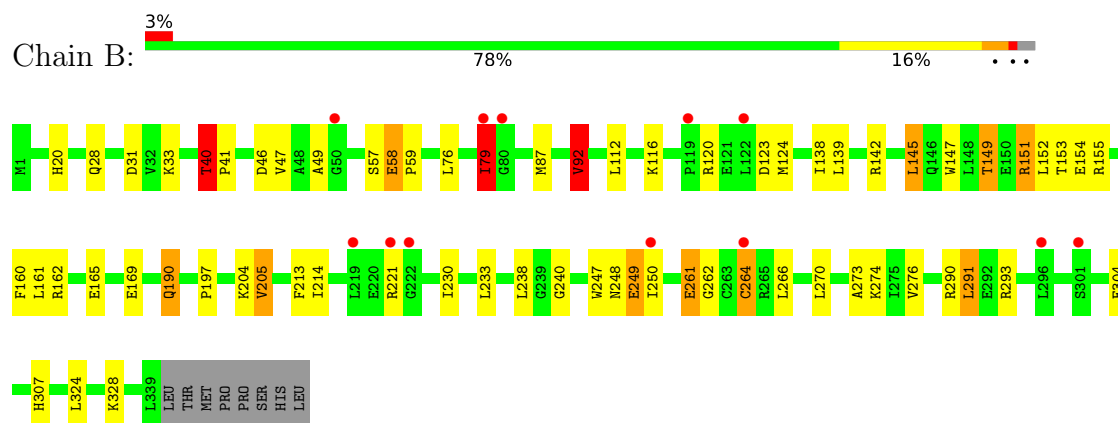
3 Residue-property plots [i](#)

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: D-amino-acid oxidase



• Molecule 1: D-amino-acid oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.62Å 91.61Å 110.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.13 – 1.88 34.13 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.2 (34.13-1.88) 97.7 (34.13-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.188 , 0.230 0.198 , 0.236	Depositor DCC
R_{free} test set	2860 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5753	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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: SO4, FAD, QSC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	0/2799	0.98	6/3813 (0.2%)
1	B	0.78	1/2784 (0.0%)	0.95	7/3792 (0.2%)
All	All	0.77	1/5583 (0.0%)	0.96	13/7605 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	CYS	CA-CB	6.59	1.64	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	THR	CB-CA-C	-10.87	91.73	109.56
1	A	28	GLN	CA-C-N	-9.70	108.18	120.79
1	A	28	GLN	C-N-CA	-9.70	108.18	120.79
1	B	40	THR	CB-CA-C	-8.54	95.56	109.56
1	B	92	VAL	CB-CA-C	-7.60	97.10	110.71
1	B	276	VAL	CB-CA-C	-6.79	103.74	111.55
1	A	94	GLY	N-CA-C	6.18	119.51	110.80
1	A	40	THR	OG1-CB-CG2	5.85	121.00	109.30
1	B	79	ILE	N-CA-C	5.77	115.96	110.42
1	B	264	CYS	N-CA-C	-5.46	105.49	111.82
1	B	190	GLN	CA-C-N	-5.35	114.25	119.76
1	B	190	GLN	C-N-CA	-5.35	114.25	119.76
1	A	40	THR	N-CA-CB	5.21	117.41	109.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2724	0	2685	48	1
1	B	2709	0	2667	42	1
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	9	0	11	1	0
3	B	9	0	11	1	0
4	A	10	0	0	3	0
4	B	10	0	0	0	0
5	A	94	0	0	4	0
5	B	82	0	0	6	0
All	All	5753	0	5436	91	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 8.

All (91) 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:79:ILE:HG21	1:B:124:MET:HE3	1.40	0.99
1:A:143:LYS:HE2	5:A:592:HOH:O	1.68	0.94
1:B:293:ARG:HG2	1:B:304:GLU:OE2	1.74	0.88
1:B:40:THR:HG23	1:B:46:ASP:OD2	1.79	0.82
1:B:145:LEU:O	1:B:149:THR:HG23	1.85	0.76
1:B:92:VAL:HG22	1:B:138:ILE:HG12	1.69	0.75
1:A:20:HIS:HD2	1:A:155:ARG:HE	1.34	0.74
1:A:20:HIS:CD2	1:A:155:ARG:HE	2.07	0.72
1:A:40:THR:HG23	1:A:46:ASP:OD2	1.90	0.72
1:B:205:VAL:HG13	1:B:273:ALA:HB1	1.74	0.69
1:B:49:ALA:HB1	1:B:230:ILE:HD12	1.76	0.67
1:B:40:THR:CG2	1:B:46:ASP:OD2	2.43	0.67
1:A:145:LEU:O	1:A:149:THR:HG23	1.96	0.65
1:B:33:LYS:HD2	1:B:160:PHE:HE2	1.60	0.65
1:A:143:LYS:CE	5:A:592:HOH:O	2.36	0.65
1:A:172:ARG:HD3	5:A:542:HOH:O	1.96	0.65
1:B:92:VAL:CG2	1:B:138:ILE:HG12	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:HIS:CD2	1:A:155:ARG:HH21	2.17	0.62
1:B:20:HIS:HD2	1:B:155:ARG:HE	1.47	0.61
1:A:20:HIS:HD2	1:A:155:ARG:NE	1.97	0.61
1:A:190:GLN:HE22	1:A:290:ARG:HH22	1.48	0.60
1:A:79:ILE:CG2	1:B:124:MET:HE3	2.24	0.60
1:B:145:LEU:O	1:B:149:THR:CG2	2.50	0.60
1:A:120:ARG:HD3	4:A:404:SO4:S	2.42	0.59
1:B:293:ARG:CG	1:B:304:GLU:OE2	2.47	0.59
1:A:28:GLN:HB3	1:A:29:PRO:HD3	1.83	0.59
1:B:190:GLN:HE22	1:B:290:ARG:HH22	1.51	0.58
1:A:1:MET:HA	1:A:1:MET:HE2	1.85	0.58
1:A:248:ASN:C	1:A:248:ASN:HD22	2.12	0.58
1:B:40:THR:CG2	1:B:142:ARG:HH11	2.17	0.58
1:A:40:THR:CG2	1:A:142:ARG:HH11	2.17	0.57
1:A:20:HIS:HD2	1:A:155:ARG:HH21	1.51	0.57
1:A:78:HIS:O	1:A:81:SER:HB3	2.06	0.56
1:A:149:THR:HG21	5:A:555:HOH:O	2.06	0.55
1:B:261:GLU:HG3	1:B:262:GLY:N	2.22	0.55
1:A:218:ASP:OD2	1:A:221:ARG:NH1	2.41	0.53
1:A:104:ASP:OD1	1:A:116:LYS:HE3	2.07	0.53
1:A:40:THR:CG2	1:A:46:ASP:OD2	2.56	0.53
1:B:58:GLU:HB2	1:B:59:PRO:HD2	1.90	0.52
1:A:20:HIS:HD2	1:A:155:ARG:NH2	2.08	0.52
1:B:40:THR:HG22	1:B:41:PRO:HA	1.91	0.52
1:B:291:LEU:HA	1:B:307:HIS:O	2.09	0.52
1:B:87:MET:HG2	1:B:147:TRP:CE2	2.45	0.52
1:A:295:GLN:HG3	1:A:304:GLU:OE2	2.10	0.52
1:B:204:LYS:HE3	5:B:557:HOH:O	2.10	0.51
1:B:249:GLU:O	1:B:249:GLU:HG2	2.10	0.51
1:B:153:THR:HG23	5:B:553:HOH:O	2.11	0.50
1:A:116:LYS:N	1:A:116:LYS:HD3	2.26	0.50
1:A:40:THR:HG22	1:A:41:PRO:HA	1.93	0.49
1:B:197:PRO:HG3	1:B:247:TRP:CE2	2.48	0.49
1:A:291:LEU:HA	1:A:307:HIS:O	2.13	0.49
1:B:162:ARG:CG	5:B:580:HOH:O	2.62	0.48
1:A:145:LEU:O	1:A:149:THR:CG2	2.61	0.47
1:B:31:ASP:OD2	1:B:33:LYS:HE3	2.13	0.47
1:A:87:MET:HG2	1:A:147:TRP:CE2	2.49	0.47
2:A:401:FAD:N5	3:A:402:QSC:HCL	2.30	0.47
1:A:28:GLN:HB3	1:A:29:PRO:CD	2.44	0.46
1:B:213:PHE:C	1:B:214:ILE:HG13	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:HIS:CD2	1:B:155:ARG:HE	2.29	0.46
1:A:248:ASN:ND2	1:A:250:ILE:H	2.13	0.45
1:B:149:THR:HG21	5:B:539:HOH:O	2.16	0.45
1:B:151:ARG:NH2	1:B:154:GLU:OE2	2.49	0.45
1:A:105:PRO:HD3	1:A:132:TRP:CZ2	2.52	0.45
1:A:28:GLN:CD	1:A:28:GLN:C	2.84	0.45
1:B:49:ALA:CB	1:B:230:ILE:HD12	2.44	0.44
1:A:40:THR:HG22	1:A:142:ARG:HH11	1.83	0.44
1:B:162:ARG:HG3	5:B:580:HOH:O	2.17	0.44
1:A:248:ASN:C	1:A:248:ASN:ND2	2.76	0.44
1:B:151:ARG:HH21	1:B:154:GLU:CD	2.26	0.44
1:A:120:ARG:CD	4:A:404:SO4:O2	2.66	0.43
1:B:40:THR:CG2	1:B:142:ARG:HD2	2.49	0.43
1:B:79:ILE:HD13	1:B:79:ILE:HA	1.62	0.43
1:A:20:HIS:HD2	1:A:155:ARG:CZ	2.31	0.43
1:B:20:HIS:HD2	1:B:155:ARG:NE	2.15	0.43
1:A:20:HIS:CD2	1:A:155:ARG:NH2	2.86	0.42
1:B:190:GLN:NE2	1:B:290:ARG:HH12	2.18	0.42
1:B:153:THR:CG2	5:B:553:HOH:O	2.66	0.42
1:B:197:PRO:HG3	1:B:247:TRP:CD2	2.55	0.42
1:B:40:THR:HG22	1:B:142:ARG:HH11	1.85	0.42
2:B:401:FAD:H9	2:B:401:FAD:H1'1	1.75	0.41
1:A:293:ARG:HD2	1:A:304:GLU:OE2	2.20	0.41
1:A:293:ARG:HD2	1:A:304:GLU:CG	2.50	0.41
3:B:402:QSC:HBE	3:B:402:QSC:HAE	1.82	0.41
1:A:69:GLN:NE2	1:A:110:MET:HG2	2.36	0.41
1:A:223:ILE:HD12	1:A:224:TYR:CE2	2.56	0.41
1:A:120:ARG:HD2	4:A:404:SO4:O2	2.22	0.40
1:A:248:ASN:HD22	1:A:250:ILE:H	1.67	0.40
1:B:248:ASN:HD22	1:B:250:ILE:H	1.69	0.40
1:A:1:MET:HE2	1:A:1:MET:CA	2.50	0.40
1:A:89:LEU:HA	1:A:138:ILE:O	2.22	0.40
1:A:166:SER:O	1:A:169:GLU:HG2	2.21	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:99:ARG:NH1	1:B:123:ASP:OD1[4_555]	2.17	0.03

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	339/347 (98%)	327 (96%)	12 (4%)	0	100	100
1	B	337/347 (97%)	326 (97%)	10 (3%)	1 (0%)	36	26
All	All	676/694 (97%)	653 (97%)	22 (3%)	1 (0%)	48	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	240	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	291/297 (98%)	260 (89%)	31 (11%)	6	1
1	B	289/297 (97%)	257 (89%)	32 (11%)	6	0
All	All	580/594 (98%)	517 (89%)	63 (11%)	6	1

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	27	LEU
1	A	40	THR
1	A	60	SER
1	A	76	LEU

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Mol	Chain	Res	Type
1	A	112	LEU
1	A	116	LYS
1	A	129	ARG
1	A	139	LEU
1	A	143	LYS
1	A	145	LEU
1	A	149	THR
1	A	151	ARG
1	A	152	LEU
1	A	161	LEU
1	A	162	ARG
1	A	165	GLU
1	A	206	ASP
1	A	223	ILE
1	A	238	LEU
1	A	244	VAL
1	A	248	ASN
1	A	254	GLN
1	A	266	LEU
1	A	270	LEU
1	A	291	LEU
1	A	301	SER
1	A	324	LEU
1	A	328	LYS
1	A	332	LYS
1	A	334	LEU
1	B	28	GLN
1	B	40	THR
1	B	47	VAL
1	B	57	SER
1	B	58	GLU
1	B	76	LEU
1	B	79	ILE
1	B	92	VAL
1	B	112	LEU
1	B	116	LYS
1	B	120	ARG
1	B	139	LEU
1	B	145	LEU
1	B	149	THR
1	B	151	ARG
1	B	152	LEU

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Mol	Chain	Res	Type
1	B	161	LEU
1	B	165	GLU
1	B	169	GLU
1	B	205	VAL
1	B	221	ARG
1	B	233	LEU
1	B	238	LEU
1	B	249	GLU
1	B	261	GLU
1	B	264	CYS
1	B	266	LEU
1	B	270	LEU
1	B	274	LYS
1	B	291	LEU
1	B	324	LEU
1	B	328	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	66	ASN
1	A	69	GLN
1	A	70	GLN
1	A	146	GLN
1	A	190	GLN
1	A	243	GLN
1	A	248	ASN
1	B	20	HIS
1	B	190	GLN
1	B	212	ASN
1	B	248	ASN
1	B	295	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
4	SO4	A	403	-	4,4,4	0.46	0	6,6,6	0.51	0
3	QSC	A	402	-	9,9,9	2.41	1 (11%)	11,11,11	0.81	0
4	SO4	B	403	-	4,4,4	0.59	0	6,6,6	0.34	0
4	SO4	A	404	-	4,4,4	0.45	0	6,6,6	0.57	0
4	SO4	B	404	-	4,4,4	0.49	0	6,6,6	0.30	0
2	FAD	A	401	-	58,58,58	1.49	10 (17%)	85,89,89	1.57	13 (15%)
2	FAD	B	401	-	58,58,58	1.42	9 (15%)	85,89,89	1.49	13 (15%)
3	QSC	B	402	-	9,9,9	2.31	1 (11%)	11,11,11	0.87	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
3	QSC	B	402	-	-	1/4/4/4	0/1/1/1
2	FAD	B	401	-	-	0/34/50/50	0/6/6/6
2	FAD	A	401	-	-	1/34/50/50	0/6/6/6
3	QSC	A	402	-	-	1/4/4/4	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	QSC	CCI-CCL	-7.08	1.41	1.52
3	B	402	QSC	CCI-CCL	-6.77	1.41	1.52
2	A	401	FAD	C9A-C5X	5.40	1.49	1.41
2	B	401	FAD	C9A-C5X	4.24	1.48	1.41
2	A	401	FAD	C5A-C4A	3.47	1.45	1.39
2	B	401	FAD	C5A-C4A	3.27	1.44	1.39
2	B	401	FAD	P-O3P	3.12	1.62	1.59
2	A	401	FAD	C4A-N9A	-3.12	1.31	1.37
2	A	401	FAD	C8-C7	2.87	1.47	1.40
2	B	401	FAD	C8-C7	2.68	1.47	1.40
2	A	401	FAD	C8A-N7A	2.63	1.36	1.31
2	A	401	FAD	C4X-N5	2.57	1.36	1.30
2	B	401	FAD	C5X-N5	-2.51	1.34	1.39
2	A	401	FAD	C5A-N7A	-2.46	1.34	1.39
2	B	401	FAD	C4A-N9A	-2.42	1.32	1.37
2	B	401	FAD	C4-N3	-2.40	1.34	1.38
2	A	401	FAD	C4-N3	-2.29	1.34	1.38
2	B	401	FAD	C4X-N5	2.24	1.35	1.30
2	B	401	FAD	C5A-N7A	-2.23	1.35	1.39
2	A	401	FAD	C5A-C6A	2.21	1.47	1.41
2	A	401	FAD	C5X-N5	-2.13	1.35	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FAD	C5A-C4A-N3A	-4.89	119.98	126.72
2	A	401	FAD	C4A-N9A-C8A	4.64	110.61	105.74
2	A	401	FAD	N3A-C4A-N9A	4.50	134.82	127.17
2	B	401	FAD	C5A-C4A-N3A	-4.41	120.65	126.72
2	B	401	FAD	N3A-C2A-N1A	-3.85	122.75	128.58
2	B	401	FAD	N3A-C4A-N9A	3.69	133.44	127.17
2	B	401	FAD	C4A-N9A-C8A	3.42	109.33	105.74
2	A	401	FAD	C2A-N3A-C4A	3.30	119.90	111.83
2	A	401	FAD	N9A-C8A-N7A	-3.28	109.29	113.94
2	B	401	FAD	C2A-N3A-C4A	3.20	119.64	111.83
2	A	401	FAD	N3A-C2A-N1A	-3.05	123.97	128.58
2	B	401	FAD	C4A-C5A-N7A	-3.03	107.11	110.58
2	A	401	FAD	C4-C4X-N5	3.03	122.39	118.21
2	A	401	FAD	O2A-PA-O1A	2.48	123.98	112.44
2	B	401	FAD	N9A-C8A-N7A	-2.45	110.47	113.94
2	A	401	FAD	C4X-C10-N10	2.42	119.95	116.48
2	B	401	FAD	N6A-C6A-N1A	2.40	123.73	118.38
2	B	401	FAD	C4-C4X-N5	2.37	121.48	118.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	FAD	C5A-N7A-C8A	2.36	107.16	103.45
2	A	401	FAD	C2B-C1B-N9A	2.25	118.90	113.30
2	B	401	FAD	C2A-N1A-C6A	2.20	122.35	118.73
2	A	401	FAD	C4-N3-C2	-2.18	121.77	125.64
2	B	401	FAD	O2P-P-O1P	2.15	122.45	112.44
2	A	401	FAD	C4X-C4-N3	2.12	118.66	113.25
2	A	401	FAD	C3B-C2B-C1B	-2.12	97.46	101.46
2	B	401	FAD	C4X-C10-N1	-2.02	119.63	124.59

There are no chirality outliers.

All (3) torsion outliers are listed below:

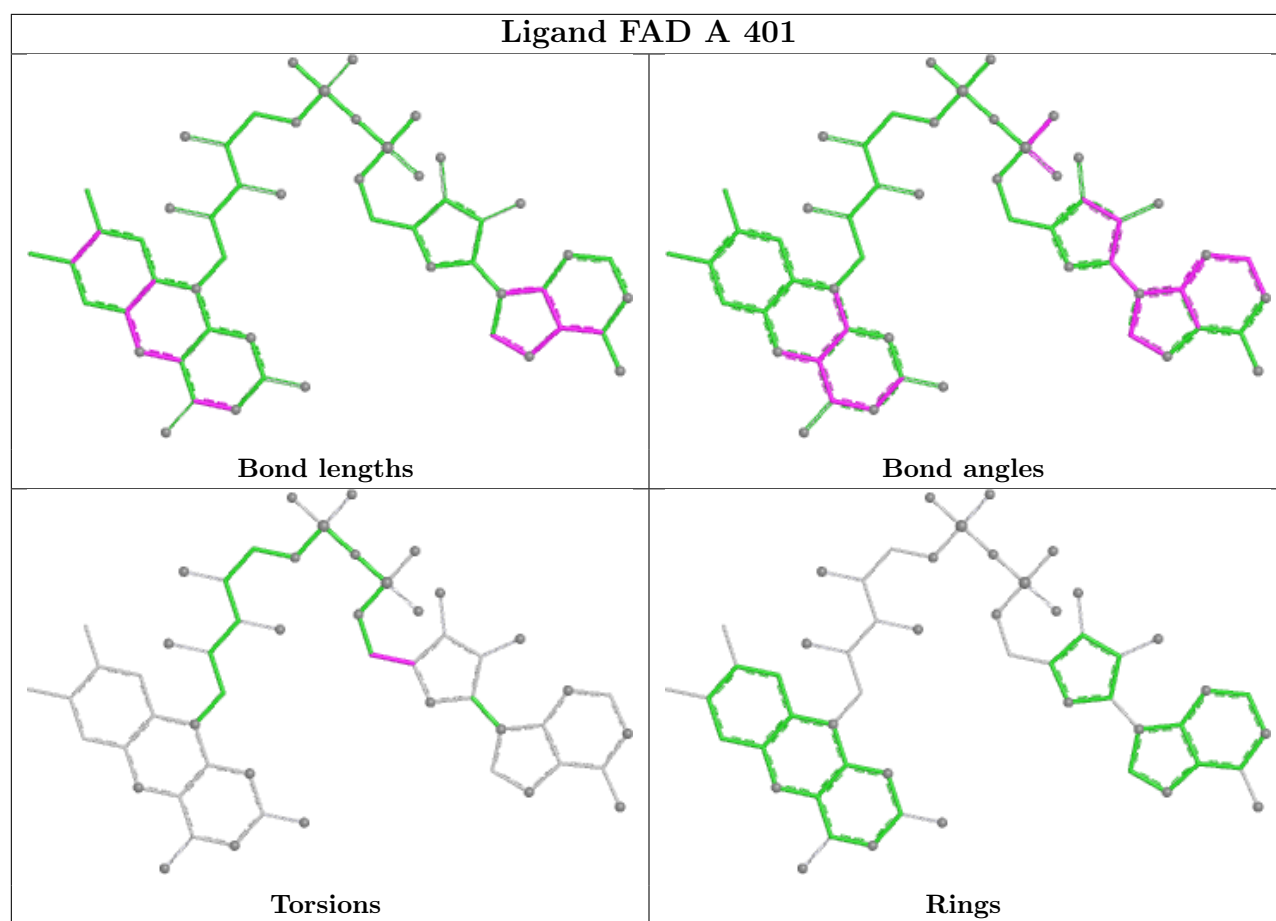
Mol	Chain	Res	Type	Atoms
3	A	402	QSC	CBF-CCI-CCL-CAE
3	B	402	QSC	CBF-CCI-CCL-CAE
2	A	401	FAD	O4B-C4B-C5B-O5B

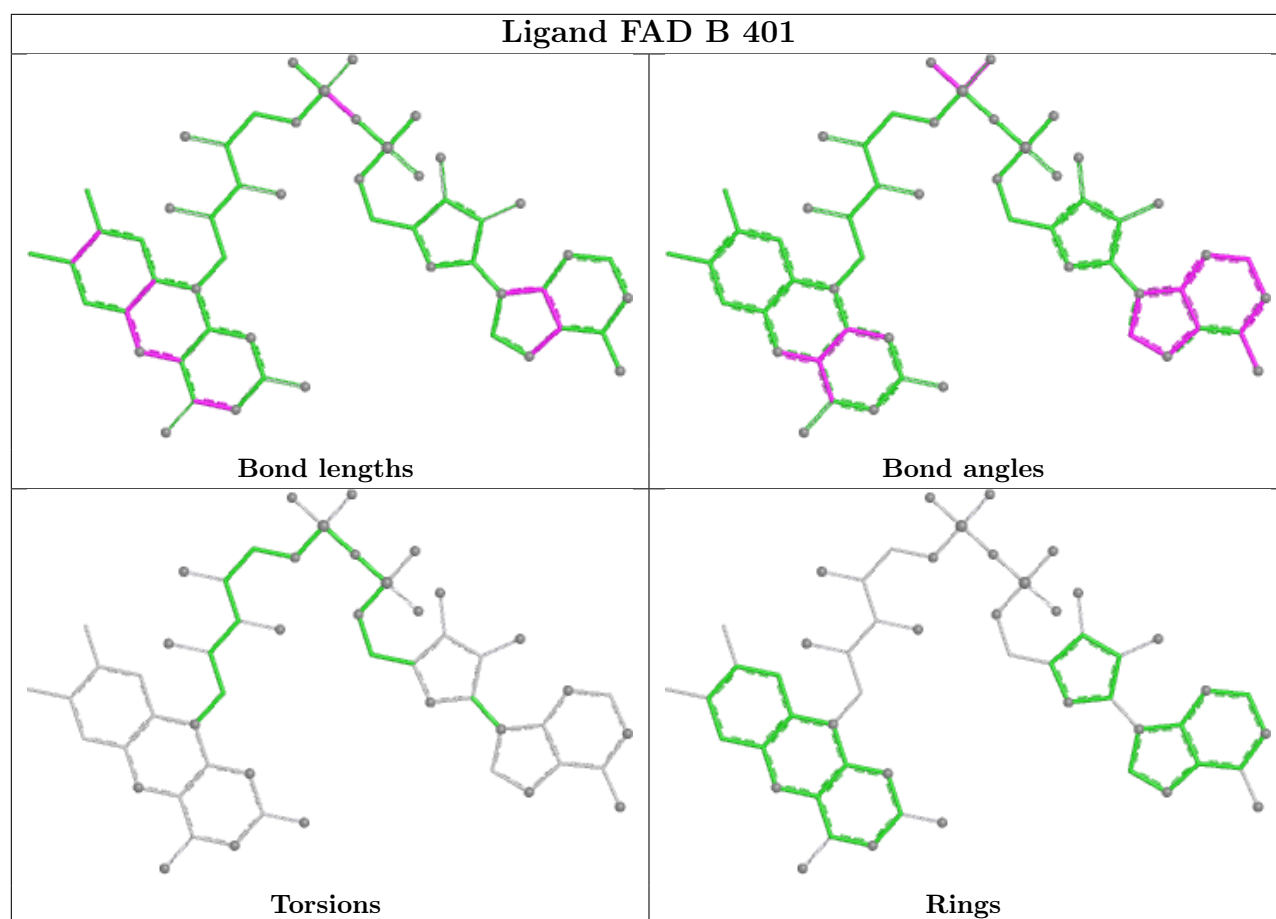
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	QSC	1	0
4	A	404	SO4	3	0
2	A	401	FAD	1	0
2	B	401	FAD	1	0
3	B	402	QSC	1	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	341/347 (98%)	0.24	17 (4%) 34 36	15, 25, 46, 69	0
1	B	339/347 (97%)	0.28	12 (3%) 47 52	16, 25, 46, 62	0
All	All	680/694 (97%)	0.26	29 (4%) 40 43	15, 25, 46, 69	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	GLY	3.7
1	A	250	ILE	3.3
1	A	253	ILE	3.3
1	B	122	LEU	3.3
1	A	1	MET	3.1
1	A	264	CYS	3.1
1	B	264	CYS	3.0
1	A	28	GLN	2.9
1	A	29	PRO	2.9
1	A	49	ALA	2.9
1	B	221	ARG	2.8
1	A	50	GLY	2.8
1	B	119	PRO	2.6
1	B	80	GLY	2.6
1	A	299	GLY	2.5
1	B	250	ILE	2.4
1	A	275	ILE	2.4
1	B	79	ILE	2.4
1	B	296	LEU	2.3
1	A	341	THR	2.3
1	B	222	GLY	2.2
1	B	301	SER	2.2
1	A	128	TYR	2.2
1	A	276	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	248	ASN	2.1
1	A	301	SER	2.1
1	A	221	ARG	2.1
1	A	338	ASN	2.0
1	B	219	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

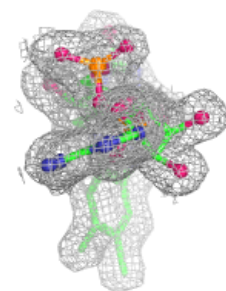
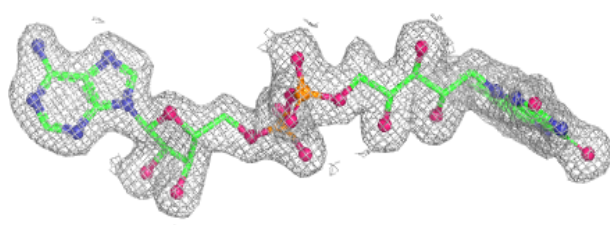
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	QSC	B	402	9/9	0.89	0.10	25,26,32,32	0
4	SO4	B	403	5/5	0.91	0.12	36,41,47,50	0
4	SO4	A	404	5/5	0.92	0.10	37,39,44,46	0
3	QSC	A	402	9/9	0.92	0.09	24,25,28,30	0
4	SO4	B	404	5/5	0.96	0.08	30,30,36,38	0
2	FAD	A	401	53/53	0.98	0.05	14,17,20,23	0
2	FAD	B	401	53/53	0.98	0.05	15,19,24,25	0
4	SO4	A	403	5/5	0.98	0.10	25,28,33,33	0

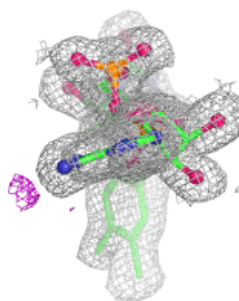
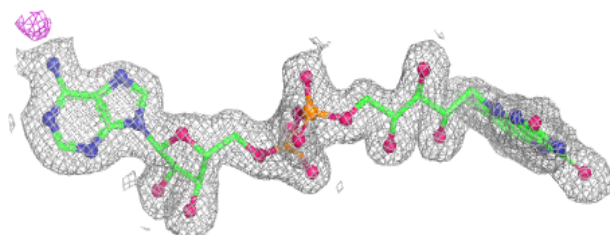
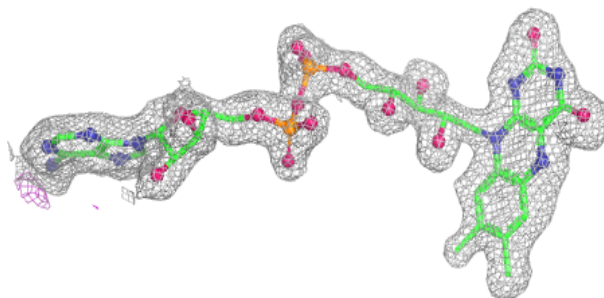
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 401:

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

**Electron density around FAD B 401:**

$2mF_o-DF_c$ (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.