



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:57 AM UTC

PDB ID : 4K2X / pdb_00004k2x
Title : OxyS anhydrotetracycline hydroxylase from *Streptomyces rimosus*
Authors : Wang, P.; Sawaya, M.R.; Tang, Y.
Deposited on : 2013-04-09
Resolution : 2.55 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

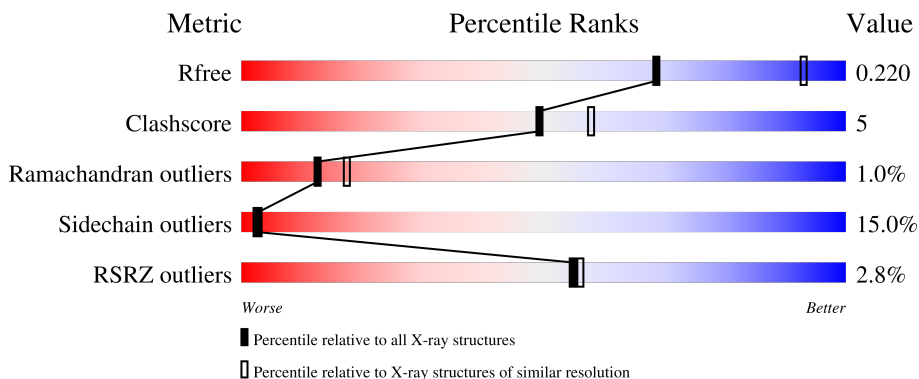
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	523	3% 70% 20% • 7%
1	B	523	2% 72% 17% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7588 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 Polyketide oxygenase/hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3712	2344	658	696	14			
1	B	490	Total	C	N	O	S	0	0	0
			3722	2350	660	698	14			

There are 40 discrepancies between the modelled and reference sequences:

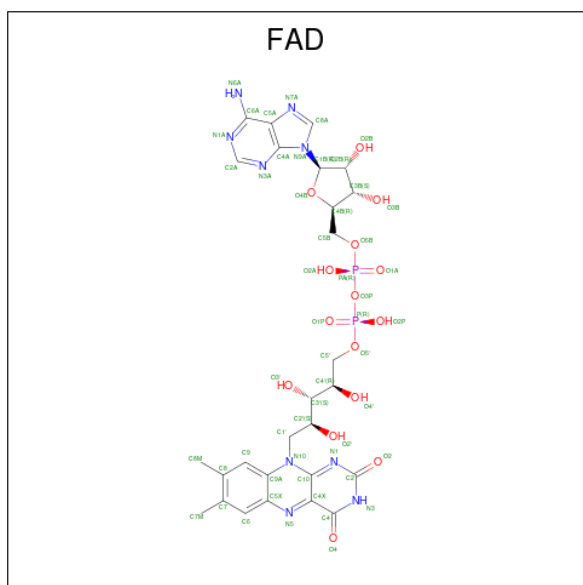
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP L8EUQ6
A	-18	GLY	-	expression tag	UNP L8EUQ6
A	-17	SER	-	expression tag	UNP L8EUQ6
A	-16	SER	-	expression tag	UNP L8EUQ6
A	-15	HIS	-	expression tag	UNP L8EUQ6
A	-14	HIS	-	expression tag	UNP L8EUQ6
A	-13	HIS	-	expression tag	UNP L8EUQ6
A	-12	HIS	-	expression tag	UNP L8EUQ6
A	-11	HIS	-	expression tag	UNP L8EUQ6
A	-10	HIS	-	expression tag	UNP L8EUQ6
A	-9	SER	-	expression tag	UNP L8EUQ6
A	-8	SER	-	expression tag	UNP L8EUQ6
A	-7	GLY	-	expression tag	UNP L8EUQ6
A	-6	LEU	-	expression tag	UNP L8EUQ6
A	-5	VAL	-	expression tag	UNP L8EUQ6
A	-4	PRO	-	expression tag	UNP L8EUQ6
A	-3	ARG	-	expression tag	UNP L8EUQ6
A	-2	GLY	-	expression tag	UNP L8EUQ6
A	-1	SER	-	expression tag	UNP L8EUQ6
A	0	HIS	-	expression tag	UNP L8EUQ6
B	-19	MET	-	expression tag	UNP L8EUQ6
B	-18	GLY	-	expression tag	UNP L8EUQ6
B	-17	SER	-	expression tag	UNP L8EUQ6
B	-16	SER	-	expression tag	UNP L8EUQ6
B	-15	HIS	-	expression tag	UNP L8EUQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP L8EUQ6
B	-13	HIS	-	expression tag	UNP L8EUQ6
B	-12	HIS	-	expression tag	UNP L8EUQ6
B	-11	HIS	-	expression tag	UNP L8EUQ6
B	-10	HIS	-	expression tag	UNP L8EUQ6
B	-9	SER	-	expression tag	UNP L8EUQ6
B	-8	SER	-	expression tag	UNP L8EUQ6
B	-7	GLY	-	expression tag	UNP L8EUQ6
B	-6	LEU	-	expression tag	UNP L8EUQ6
B	-5	VAL	-	expression tag	UNP L8EUQ6
B	-4	PRO	-	expression tag	UNP L8EUQ6
B	-3	ARG	-	expression tag	UNP L8EUQ6
B	-2	GLY	-	expression tag	UNP L8EUQ6
B	-1	SER	-	expression tag	UNP L8EUQ6
B	0	HIS	-	expression tag	UNP L8EUQ6

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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		

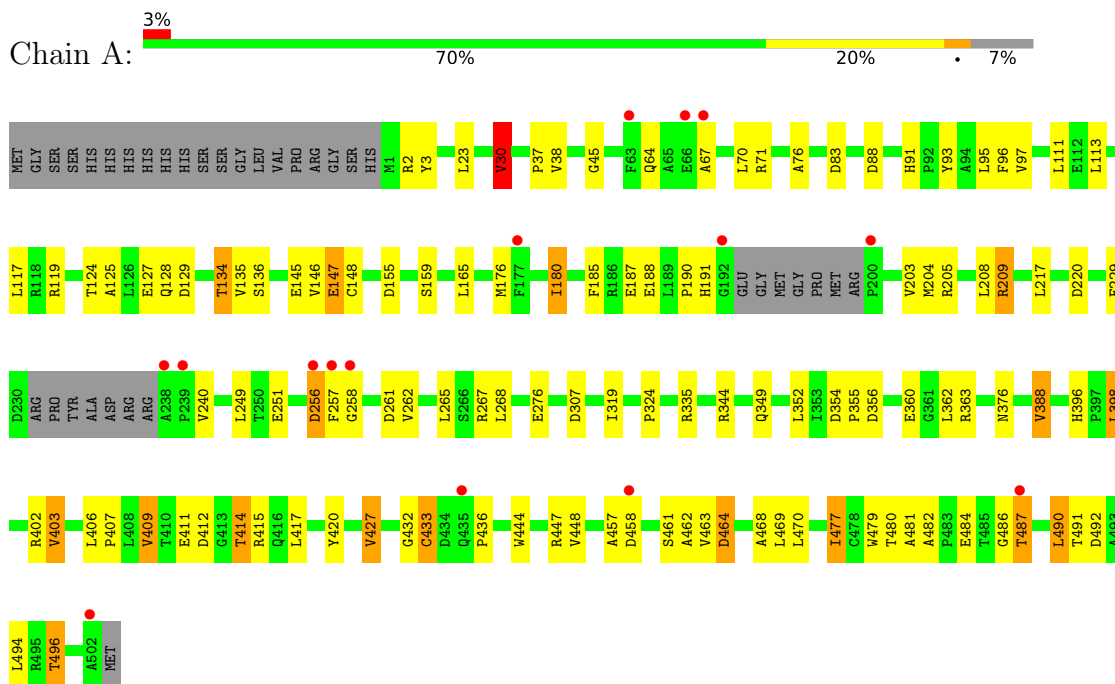
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total 23	O 23	0	0
3	B	25	Total 25	O 25	0	0

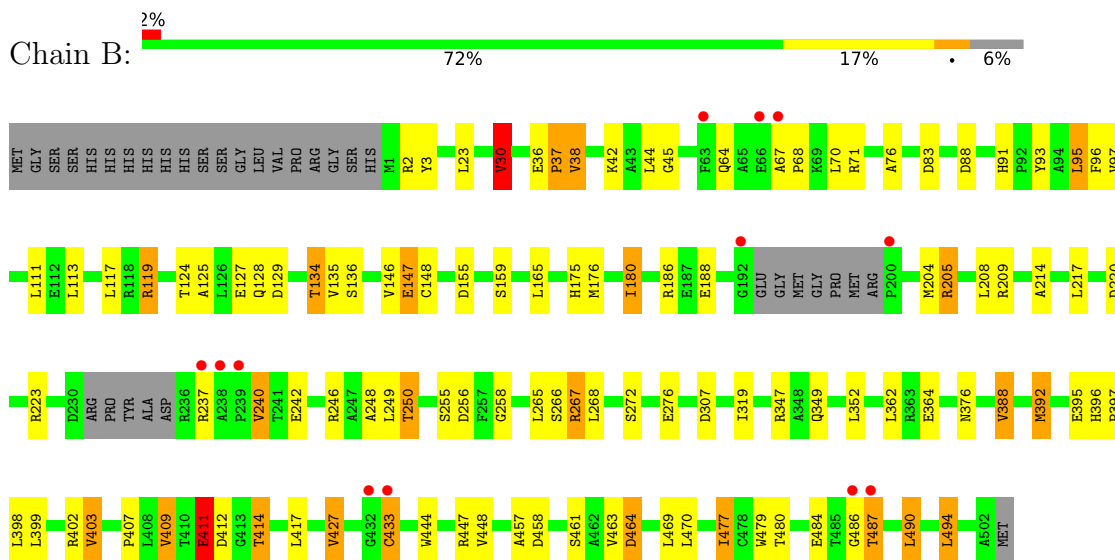
3 Residue-property plots

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: Polyketide oxygenase/hydroxylase



• Molecule 1: Polyketide oxygenase/hydroxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.06Å 115.13Å 121.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.05 – 2.55 34.05 – 2.55	Depositor EDS
% Data completeness (in resolution range)	89.0 (34.05-2.55) 89.0 (34.05-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.54Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.10.0	Depositor
R, R_{free}	0.187 , 0.229 (Not available) , 0.220	Depositor DCC
R_{free} test set	1573 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7588	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.40 % 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 3.7090e-04. 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

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	0.84	1/3795 (0.0%)	1.37	26/5169 (0.5%)
1	B	0.86	0/3805	1.37	26/5183 (0.5%)
All	All	0.85	1/7600 (0.0%)	1.37	52/10352 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	PRO	CA-C	5.56	1.55	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	VAL	N-CA-CB	8.83	120.64	110.49
1	B	411	GLU	N-CA-C	-7.49	98.37	110.20
1	B	464	ASP	N-CA-C	6.57	118.99	111.11
1	A	67	ALA	N-CA-C	6.33	123.80	109.81
1	B	392	MET	N-CA-C	-6.20	99.30	109.40
1	B	248	ALA	CA-C-N	6.18	128.48	120.44
1	B	248	ALA	C-N-CA	6.18	128.48	120.44
1	B	67	ALA	N-CA-C	6.14	123.38	109.81
1	B	403	VAL	N-CA-CB	6.09	119.73	111.21
1	A	354	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	37	PRO	CA-C-N	5.97	128.50	120.50
1	B	37	PRO	C-N-CA	5.97	128.50	120.50
1	B	307	ASP	CA-CB-CG	5.88	118.48	112.60
1	A	414	THR	CB-CA-C	5.85	119.18	109.53
1	A	490	LEU	CA-C-N	5.83	128.37	120.38
1	A	490	LEU	C-N-CA	5.83	128.37	120.38
1	A	307	ASP	CA-CB-CG	5.80	118.40	112.60
1	B	38	VAL	N-CA-CB	-5.75	100.47	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	PRO	CA-C-N	5.75	128.42	120.49
1	A	37	PRO	C-N-CA	5.75	128.42	120.49
1	B	409	VAL	CB-CA-C	5.75	117.91	110.96
1	A	462	ALA	CA-C-N	5.69	129.61	121.02
1	A	462	ALA	C-N-CA	5.69	129.61	121.02
1	B	395	GLU	N-CA-C	5.69	122.03	114.12
1	B	414	THR	CB-CA-C	5.68	118.91	109.53
1	B	409	VAL	N-CA-CB	5.64	117.43	111.00
1	A	409	VAL	N-CA-CB	5.60	117.71	110.99
1	A	464	ASP	N-CA-C	5.52	120.47	111.37
1	A	388	VAL	N-CA-CB	5.50	120.31	111.23
1	B	155	ASP	N-CA-C	5.48	119.07	112.93
1	A	403	VAL	N-CA-CB	5.48	118.88	111.21
1	A	155	ASP	N-CA-C	5.40	118.98	112.93
1	B	42	LYS	N-CA-C	-5.39	105.05	111.03
1	B	30	VAL	CB-CA-C	5.38	118.42	110.77
1	B	397	PRO	N-CA-C	5.32	120.75	113.84
1	A	482	ALA	N-CA-C	-5.28	102.47	110.50
1	B	129	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	155	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	129	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	436	PRO	CA-C-N	5.17	127.63	120.29
1	A	436	PRO	C-N-CA	5.17	127.63	120.29
1	A	444	TRP	CA-C-N	5.17	127.92	120.38
1	A	444	TRP	C-N-CA	5.17	127.92	120.38
1	A	335	ARG	N-CA-C	5.17	118.04	111.69
1	A	30	VAL	N-CA-CB	5.13	118.31	111.64
1	B	175	HIS	N-CA-C	-5.13	106.99	114.12
1	A	427	VAL	N-CA-CB	5.13	119.01	111.52
1	B	427	VAL	N-CA-CB	5.12	119.00	111.52
1	B	444	TRP	CA-C-N	5.03	127.72	120.38
1	B	444	TRP	C-N-CA	5.03	127.72	120.38
1	A	432	GLY	CA-C-N	5.01	131.11	121.54
1	A	432	GLY	C-N-CA	5.01	131.11	121.54

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	3712	0	3651	40	0
1	B	3722	0	3655	41	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
3	A	23	0	0	0	0
3	B	25	0	0	0	0
All	All	7588	0	7368	80	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 5.

All (80) 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:492:ASP:O	1:A:496:THR:HG22	1.80	0.81
1:A:362:LEU:HD21	1:B:362:LEU:HD21	1.63	0.78
1:A:477:ILE:HD11	1:A:480:THR:HG23	1.66	0.76
1:B:83:ASP:H	1:B:376:ASN:HD21	1.34	0.76
1:B:477:ILE:HD11	1:B:480:THR:HG23	1.66	0.76
1:A:83:ASP:H	1:A:376:ASN:HD21	1.35	0.74
1:A:256:ASP:OD1	1:A:256:ASP:C	2.36	0.68
1:A:76:ALA:H	1:A:349:GLN:HE21	1.41	0.66
1:B:242:GLU:OE2	1:B:246:ARG:NH1	2.29	0.65
1:B:490:LEU:HD22	1:B:494:LEU:HD22	1.77	0.65
1:A:256:ASP:OD1	1:A:258:GLY:N	2.30	0.64
1:B:30:VAL:HG22	1:B:117:LEU:HD13	1.80	0.64
1:A:469:LEU:HD23	1:A:480:THR:HG22	1.82	0.62
1:A:30:VAL:HG22	1:A:117:LEU:HD13	1.81	0.62
1:A:88:ASP:O	1:A:402:ARG:NH2	2.34	0.61
1:A:134:THR:CG2	1:A:147:GLU:HG3	2.32	0.59
1:A:76:ALA:HB2	1:A:349:GLN:HG2	1.83	0.59
1:B:469:LEU:HD23	1:B:480:THR:HG22	1.83	0.59
1:B:134:THR:CG2	1:B:147:GLU:HG3	2.32	0.59
1:B:88:ASP:O	1:B:402:ARG:NH2	2.36	0.57
1:A:256:ASP:O	1:A:257:PHE:HB2	2.04	0.56
1:A:45:GLY:HA2	1:A:97:VAL:H	1.71	0.54
1:B:45:GLY:HA2	1:B:97:VAL:H	1.72	0.54
1:A:76:ALA:H	1:A:349:GLN:NE2	2.06	0.54
1:A:180:ILE:HD11	1:A:268:LEU:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ALA:HB3	1:A:481:ALA:HB3	1.92	0.52
1:B:134:THR:HG22	1:B:147:GLU:HG3	1.90	0.52
1:A:406:LEU:HD11	1:A:463:VAL:HG21	1.91	0.52
1:A:176:MET:HE2	1:A:229:PHE:CZ	2.46	0.50
1:A:479:TRP:CH2	1:A:481:ALA:HB2	2.46	0.50
1:A:190:PRO:HD3	1:A:257:PHE:CZ	2.46	0.50
1:A:134:THR:HG22	1:A:147:GLU:HG3	1.93	0.50
1:B:407:PRO:HB2	1:B:457:ALA:HB3	1.93	0.50
1:A:415:ARG:HG2	1:A:420:TYR:CE2	2.48	0.49
1:B:237:ARG:HA	1:B:267:ARG:NH2	2.28	0.49
1:A:209:ARG:HD3	1:A:356:ASP:HB2	1.95	0.48
1:A:134:THR:HG23	1:A:147:GLU:HG3	1.96	0.48
1:B:477:ILE:HD11	1:B:480:THR:CG2	2.39	0.48
1:A:360:GLU:OE1	1:A:363:ARG:NH1	2.47	0.47
1:B:76:ALA:H	1:B:349:GLN:HE21	1.61	0.47
1:A:470:LEU:HB3	1:A:479:TRP:HB3	1.96	0.47
1:A:407:PRO:HB2	1:A:457:ALA:HB3	1.96	0.47
1:B:214:ALA:HA	1:B:223:ARG:O	2.15	0.47
1:B:396:HIS:HB2	1:B:399:LEU:HD13	1.97	0.47
1:A:477:ILE:HD11	1:A:480:THR:CG2	2.42	0.46
1:B:470:LEU:HB3	1:B:479:TRP:HB3	1.97	0.46
1:B:237:ARG:HA	1:B:267:ARG:HH22	1.81	0.46
1:B:246:ARG:O	1:B:250:THR:HB	2.16	0.46
1:B:91:HIS:HD2	1:B:93:TYR:OH	1.99	0.46
1:A:396:HIS:CE1	1:A:398:LEU:HB2	2.51	0.46
1:B:180:ILE:HD12	1:B:266:SER:HB3	1.98	0.46
1:B:240:VAL:HG21	1:B:266:SER:CA	2.45	0.46
1:B:180:ILE:HD11	1:B:268:LEU:HB2	1.98	0.46
1:B:134:THR:HG23	1:B:147:GLU:HG3	1.98	0.45
1:A:344:ARG:HE	1:B:364:GLU:HB3	1.81	0.45
1:A:70:LEU:HD11	1:A:96:PHE:HB2	1.98	0.45
1:A:91:HIS:HD2	1:A:93:TYR:OH	1.98	0.45
1:B:70:LEU:HD11	1:B:96:PHE:HB2	1.99	0.45
1:B:204:MET:O	1:B:205:ARG:HG2	2.17	0.45
1:B:2:ARG:HD2	1:B:147:GLU:HB3	1.99	0.44
1:A:2:ARG:HD2	1:A:147:GLU:HB3	1.99	0.44
1:A:125:ALA:HB3	1:A:136:SER:HB2	2.00	0.44
1:B:64:GLN:HG2	1:B:95:LEU:HD21	1.98	0.44
1:B:272:SER:HB3	1:B:347:ARG:HE	1.83	0.44
1:A:185:PHE:HD2	1:A:257:PHE:HB3	1.83	0.43
1:B:125:ALA:HB3	1:B:136:SER:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:SER:CB	1:B:347:ARG:HE	2.32	0.43
1:B:186:ARG:HB2	1:B:258:GLY:HA3	2.01	0.42
1:B:37:PRO:HG3	1:B:119:ARG:NH2	2.35	0.42
1:A:64:GLN:HG2	1:A:95:LEU:HD21	2.00	0.42
1:B:477:ILE:CD1	1:B:480:THR:HG23	2.44	0.41
1:A:477:ILE:CD1	1:A:480:THR:HG23	2.43	0.41
1:B:68:PRO:HG2	1:B:96:PHE:HB3	2.03	0.41
1:B:95:LEU:HB3	1:B:97:VAL:HG23	2.02	0.41
1:B:411:GLU:O	1:B:412:ASP:HB2	2.21	0.41
1:B:256:ASP:OD1	1:B:256:ASP:C	2.64	0.41
2:B:601:FAD:H9	2:B:601:FAD:H1'1	1.87	0.41
1:B:3:TYR:O	1:B:148:CYS:HA	2.21	0.40
1:A:204:MET:SD	1:A:355:PRO:HB3	2.62	0.40
1:A:3:TYR:O	1:A:148:CYS:HA	2.21	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	482/523 (92%)	462 (96%)	15 (3%)	5 (1%)	12	17
1	B	484/523 (92%)	465 (96%)	14 (3%)	5 (1%)	12	17
All	All	966/1046 (92%)	927 (96%)	29 (3%)	10 (1%)	12	17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	SER
1	B	461	SER
1	A	486	GLY
1	A	487	THR

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Mol	Chain	Res	Type
1	B	486	GLY
1	B	487	THR
1	A	159	SER
1	B	159	SER
1	A	433	CYS
1	B	433	CYS

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	376/405 (93%)	318 (85%)	58 (15%)	2	2
1	B	376/405 (93%)	321 (85%)	55 (15%)	3	2
All	All	752/810 (93%)	639 (85%)	113 (15%)	3	2

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	30	VAL
1	A	38	VAL
1	A	71	ARG
1	A	111	LEU
1	A	113	LEU
1	A	119	ARG
1	A	124	THR
1	A	127	GLU
1	A	128	GLN
1	A	134	THR
1	A	135	VAL
1	A	145	GLU
1	A	146	VAL
1	A	147	GLU
1	A	165	LEU
1	A	180	ILE

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Mol	Chain	Res	Type
1	A	187	GLU
1	A	188	GLU
1	A	191	HIS
1	A	203	VAL
1	A	205	ARG
1	A	208	LEU
1	A	209	ARG
1	A	217	LEU
1	A	220	ASP
1	A	240	VAL
1	A	249	LEU
1	A	251	GLU
1	A	256	ASP
1	A	261	ASP
1	A	262	VAL
1	A	265	LEU
1	A	267	ARG
1	A	276	GLU
1	A	319	ILE
1	A	352	LEU
1	A	388	VAL
1	A	398	LEU
1	A	403	VAL
1	A	409	VAL
1	A	411	GLU
1	A	412	ASP
1	A	414	THR
1	A	417	LEU
1	A	427	VAL
1	A	433	CYS
1	A	447	ARG
1	A	448	VAL
1	A	458	ASP
1	A	464	ASP
1	A	477	ILE
1	A	484	GLU
1	A	487	THR
1	A	490	LEU
1	A	491	THR
1	A	494	LEU
1	A	496	THR
1	B	23	LEU

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Mol	Chain	Res	Type
1	B	30	VAL
1	B	36	GLU
1	B	38	VAL
1	B	44	LEU
1	B	71	ARG
1	B	95	LEU
1	B	111	LEU
1	B	113	LEU
1	B	119	ARG
1	B	124	THR
1	B	127	GLU
1	B	128	GLN
1	B	134	THR
1	B	135	VAL
1	B	146	VAL
1	B	147	GLU
1	B	165	LEU
1	B	176	MET
1	B	180	ILE
1	B	188	GLU
1	B	205	ARG
1	B	208	LEU
1	B	209	ARG
1	B	217	LEU
1	B	220	ASP
1	B	240	VAL
1	B	249	LEU
1	B	250	THR
1	B	255	SER
1	B	265	LEU
1	B	267	ARG
1	B	276	GLU
1	B	319	ILE
1	B	352	LEU
1	B	388	VAL
1	B	392	MET
1	B	398	LEU
1	B	403	VAL
1	B	409	VAL
1	B	411	GLU
1	B	414	THR
1	B	417	LEU

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Mol	Chain	Res	Type
1	B	427	VAL
1	B	433	CYS
1	B	447	ARG
1	B	448	VAL
1	B	458	ASP
1	B	463	VAL
1	B	464	ASP
1	B	477	ILE
1	B	484	GLU
1	B	487	THR
1	B	490	LEU
1	B	494	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	91	HIS
1	A	349	GLN
1	A	371	HIS
1	A	376	ASN
1	A	435	GLN
1	B	64	GLN
1	B	91	HIS
1	B	206	HIS
1	B	349	GLN
1	B	371	HIS
1	B	376	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	B	601	-	58,58,58	0.58	1 (1%)	85,89,89	0.81	4 (4%)
2	FAD	A	601	-	58,58,58	0.56	1 (1%)	85,89,89	0.77	3 (3%)

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	B	601	-	-	0/34/50/50	0/6/6/6
2	FAD	A	601	-	-	0/34/50/50	0/6/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	PA-O3P	3.27	1.63	1.59
2	B	601	FAD	PA-O3P	3.23	1.63	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	O3P-P-O1P	-3.98	98.75	110.70
2	A	601	FAD	O3P-P-O1P	-3.53	100.08	110.70
2	A	601	FAD	O3P-PA-O1A	-2.32	103.72	110.70
2	B	601	FAD	O2P-P-O3P	2.26	113.37	107.27
2	B	601	FAD	O3B-C3B-C4B	-2.11	105.03	111.08
2	B	601	FAD	O3P-PA-O1A	-2.08	104.44	110.70
2	A	601	FAD	O2P-P-O3P	2.05	112.83	107.27

There are no chirality outliers.

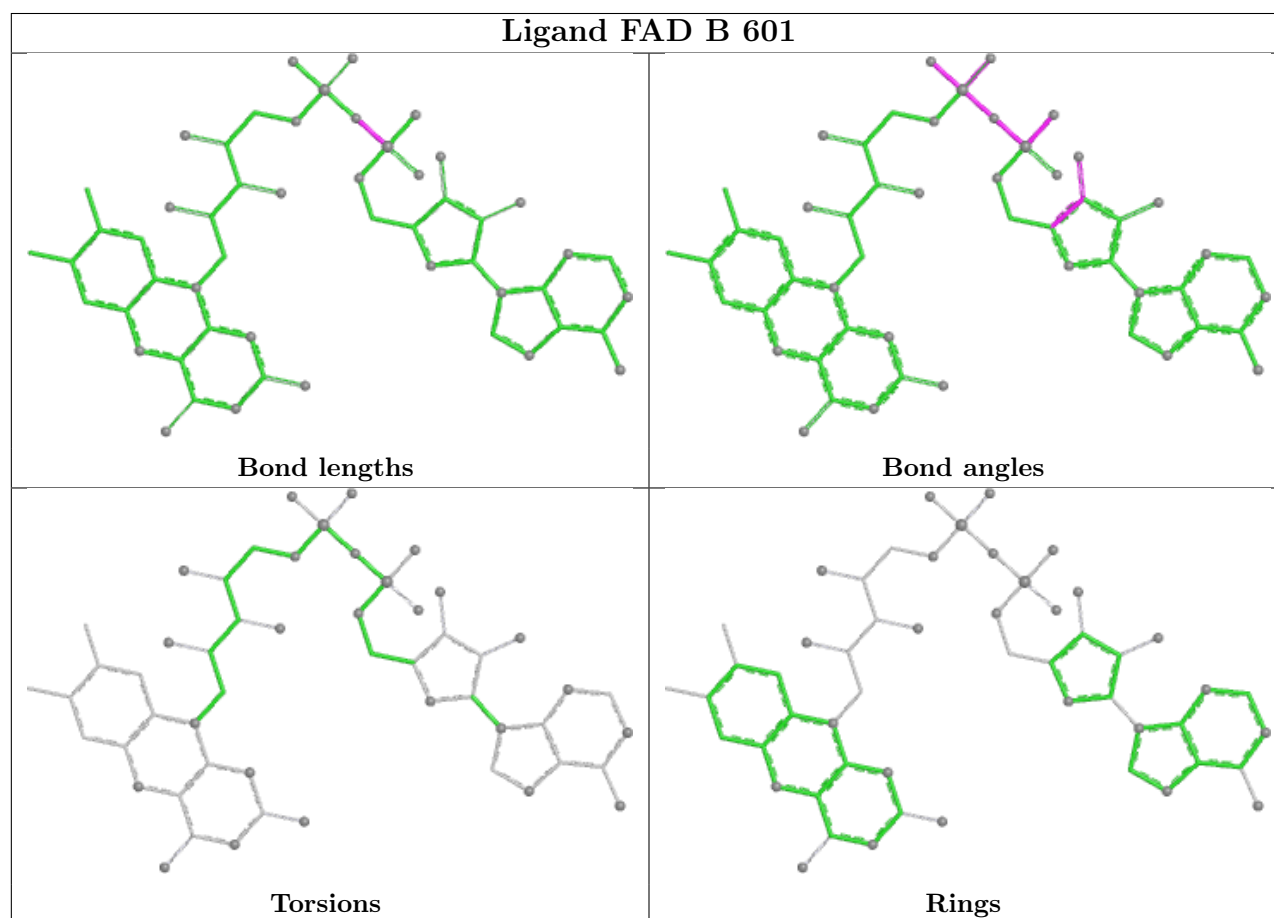
There are no torsion outliers.

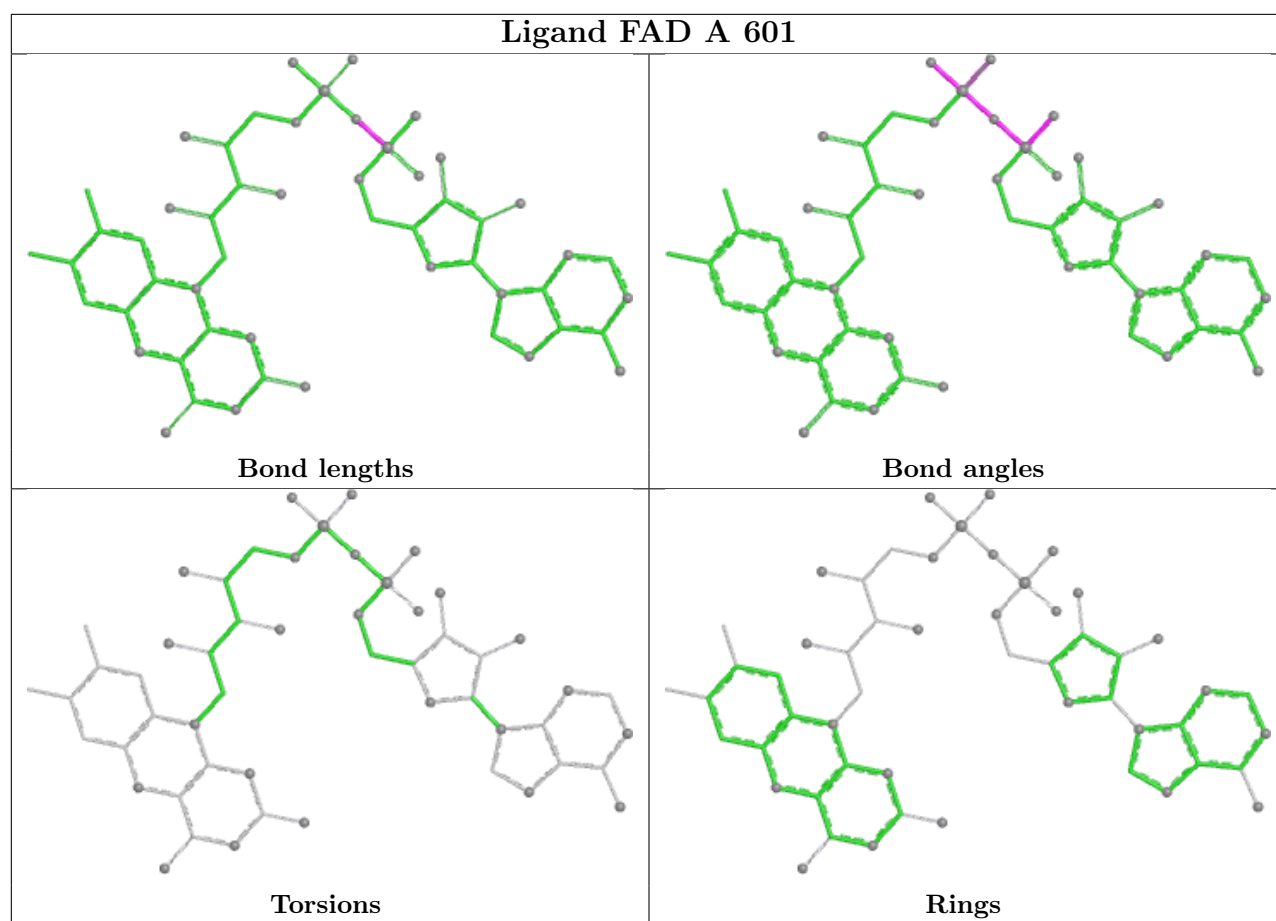
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	FAD	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	488/523 (93%)	0.04	15 (3%)	51	52	28, 46, 79, 107	0
1	B	490/523 (93%)	-0.11	12 (2%)	59	61	27, 42, 75, 104	0
All	All	978/1046 (93%)	-0.04	27 (2%)	55	56	27, 44, 78, 107	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	GLY	4.0
1	A	502	ALA	3.7
1	B	67	ALA	3.6
1	A	67	ALA	3.3
1	A	66	GLU	2.9
1	B	432	GLY	2.9
1	B	200	PRO	2.8
1	A	258	GLY	2.8
1	B	238	ALA	2.8
1	A	177	PHE	2.7
1	A	239	PRO	2.7
1	A	192	GLY	2.7
1	B	486	GLY	2.6
1	A	63	PHE	2.6
1	B	63	PHE	2.6
1	A	238	ALA	2.5
1	B	433	CYS	2.5
1	A	458	ASP	2.5
1	A	256	ASP	2.4
1	A	200	PRO	2.4
1	A	435	GLN	2.3
1	B	66	GLU	2.2
1	B	239	PRO	2.2
1	B	237	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	487	THR	2.1
1	B	487	THR	2.1
1	A	257	PHE	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](#)

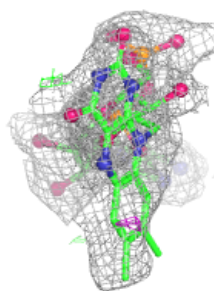
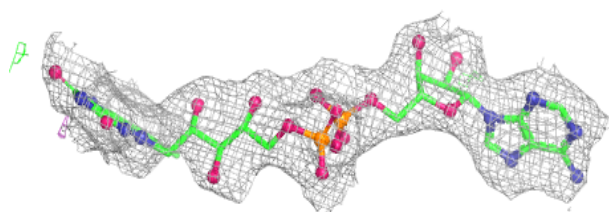
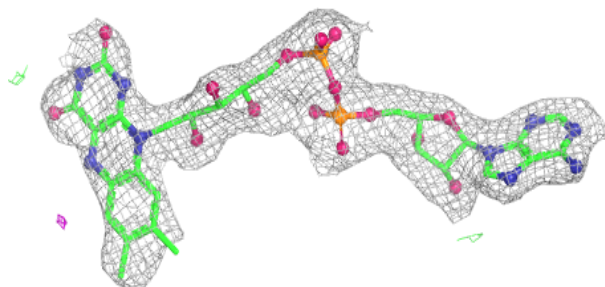
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	B	601	53/53	0.97	0.06	23,33,38,44	0
2	FAD	A	601	53/53	0.98	0.06	22,34,41,46	0

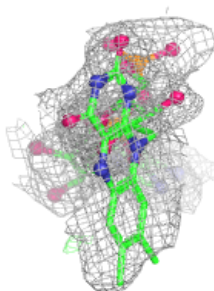
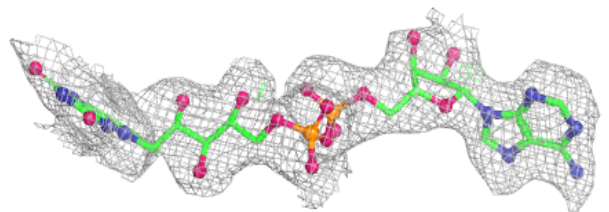
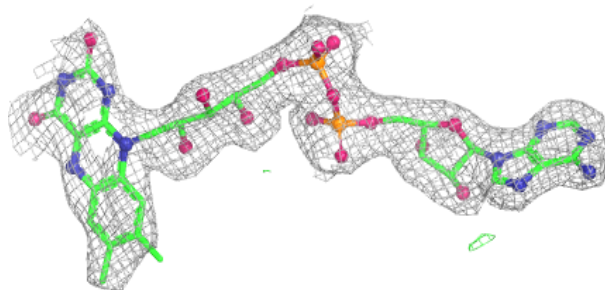
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 601:

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

**Electron density around FAD A 601:**

$2mF_o-DF_c$ (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.