



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:42 PM UTC

PDB ID : 9GOZ / pdb_00009goz
Title : 4-Allyl syringol oxidase from *Streptomyces cavernae*: complex with eugenol
Authors : Mattevi, A.; Alvigini, L.
Deposited on : 2024-09-06
Resolution : 1.40 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

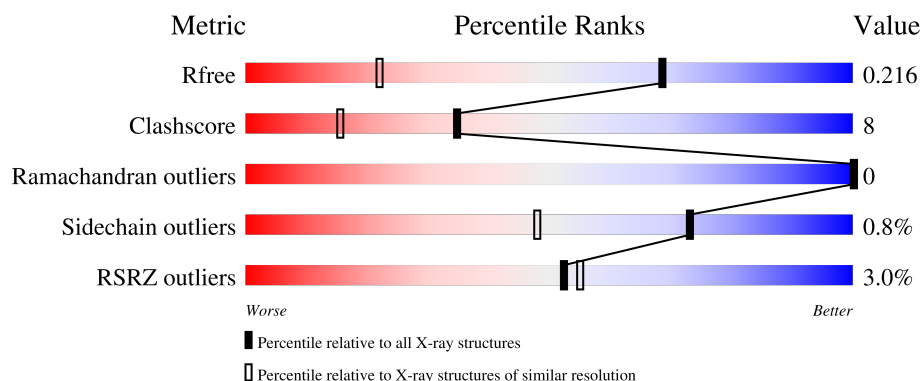
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

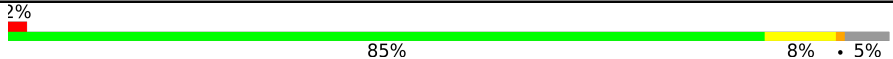
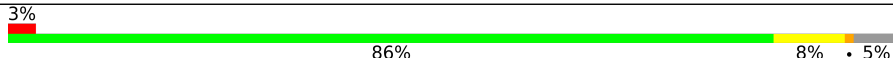
The reported resolution of this entry is 1.40 Å.

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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	554	
1	B	554	

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
5	P4G	A	604	-	-	X	-

2 Entry composition [i](#)

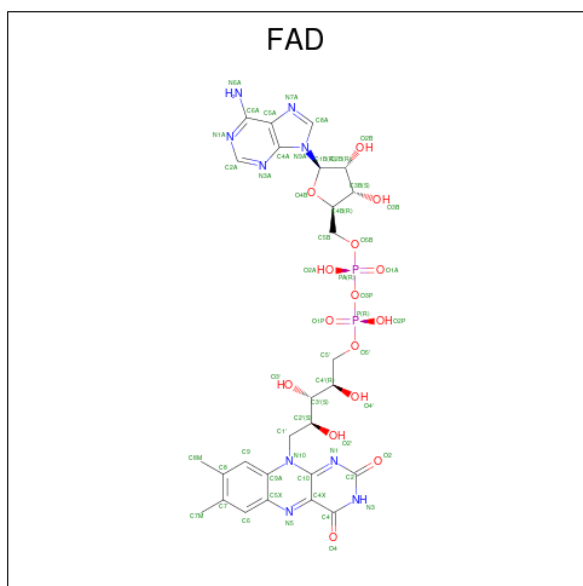
There are 7 unique types of molecules in this entry. The entry contains 9692 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4-allyl syringol oxidase from *Streptomyces cavernae*.

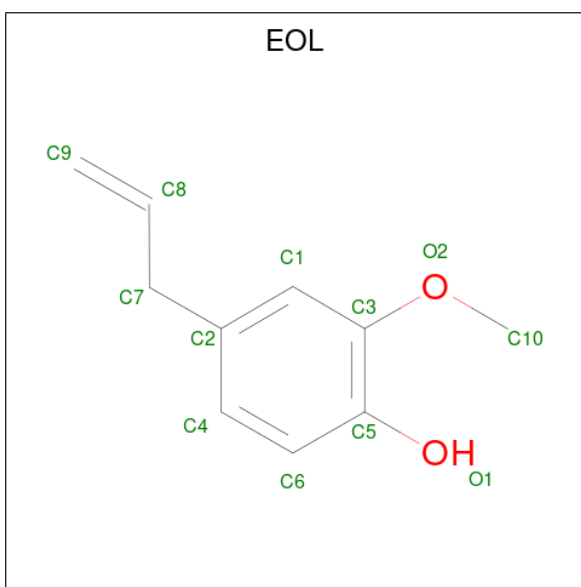
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	2	0
			4068	2581	706	759	22			
1	B	524	Total	C	N	O	S	0	0	0
			4055	2572	704	757	22			

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



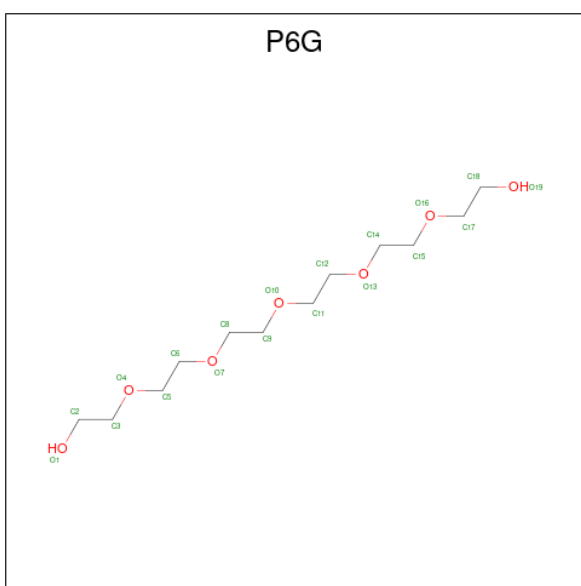
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 2-methoxy-4-(prop-2-en-1-yl)phenol (CCD ID: EOL) (formula: $C_{10}H_{12}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	10	2		
3	B	1	Total	C	O	0	0
			12	10	2		

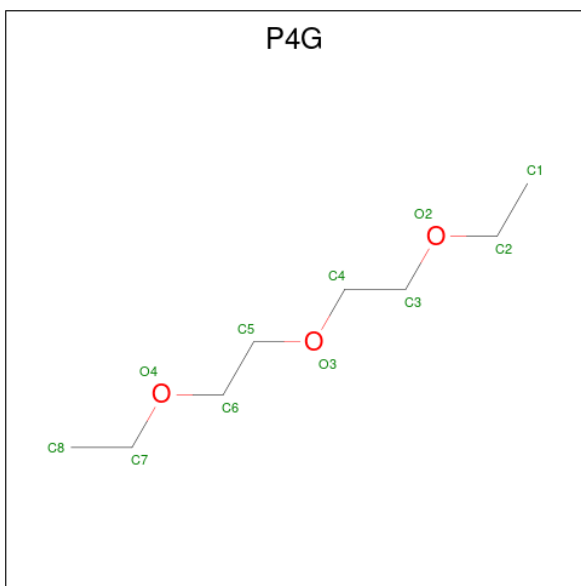
- Molecule 4 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	12	7		

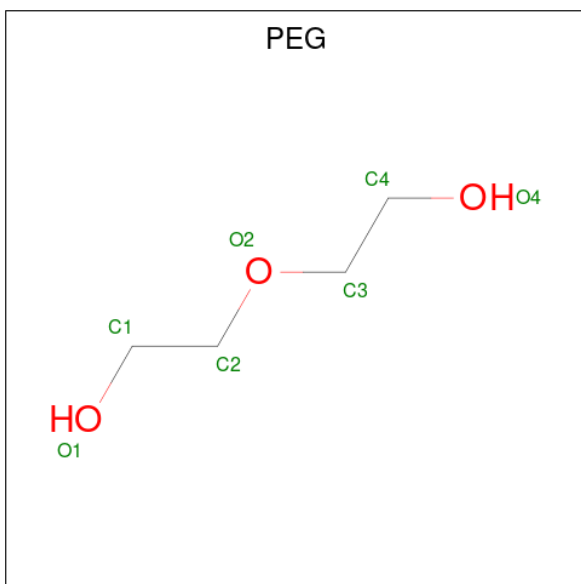
- Molecule 5 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (CCD ID: P4G) (formula:

C₈H₁₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	8	3		
5	B	1	Total	C	O	0	0
			11	8	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

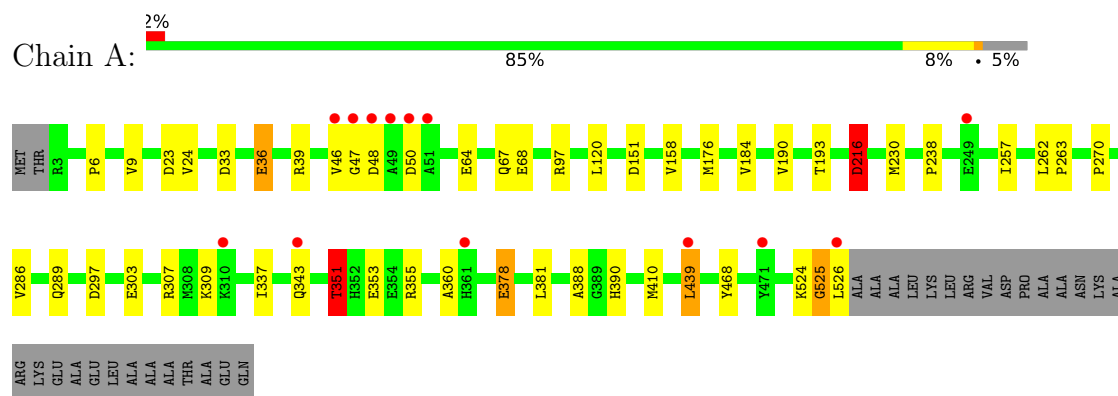
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	719	Total	O	0	0
			719	719		
7	B	658	Total	O	0	0
			658	658		

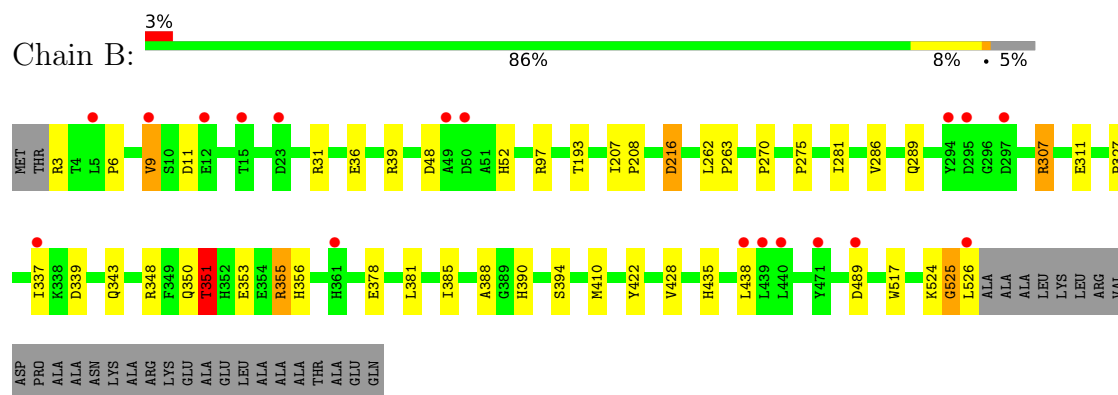
3 Residue-property plots

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: 4-allyl syringol oxidase from *Streptomyces cavernae*



- Molecule 1: 4-allyl syringol oxidase from *Streptomyces cavernae*



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	83.26Å 83.26Å 297.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.86 – 1.40 40.86 – 1.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.86-1.40) 100.0 (40.86-1.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.187 , 0.216 0.188 , 0.216	Depositor DCC
R_{free} test set	11366 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.075 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9692	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: EOL, PEG, P4G, FAD, P6G

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	1.08	4/4171 (0.1%)	1.22	17/5674 (0.3%)
1	B	1.02	2/4158 (0.0%)	1.20	6/5655 (0.1%)
All	All	1.05	6/8329 (0.1%)	1.21	23/11329 (0.2%)

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	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	VAL	CA-C	-7.14	1.44	1.52
1	B	385	ILE	C-O	-6.65	1.19	1.24
1	A	216	ASP	CG-OD2	-5.83	1.14	1.25
1	A	439	LEU	C-O	5.40	1.31	1.23
1	B	216	ASP	CG-OD2	-5.28	1.15	1.25
1	A	378	GLU	C-O	-5.12	1.17	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	VAL	N-CA-C	-12.09	90.23	108.85
1	A	46	VAL	CA-C-N	-7.47	107.11	121.01
1	A	46	VAL	C-N-CA	-7.47	107.11	121.01
1	A	64	GLU	CB-CG-CD	6.74	124.05	112.60
1	A	50	ASP	CB-CA-C	-6.52	100.64	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	GLY	O-C-N	6.14	128.43	122.41
1	A	351	THR	N-CA-CB	-5.89	101.04	110.46
1	B	351	THR	N-CA-CB	-5.80	101.17	110.46
1	A	525	GLY	CA-C-N	5.65	131.87	121.70
1	A	525	GLY	C-N-CA	5.65	131.87	121.70
1	B	388	ALA	N-CA-C	5.51	118.31	110.10
1	A	48	ASP	N-CA-C	-5.51	102.73	110.50
1	A	410	MET	CB-CA-C	-5.50	102.24	110.88
1	A	36	GLU	CB-CG-CD	5.49	121.94	112.60
1	B	410	MET	CB-CA-C	-5.32	102.53	110.88
1	A	257	ILE	N-CA-C	-5.26	105.37	110.42
1	A	468	TYR	CA-C-N	5.25	126.64	120.71
1	A	468	TYR	C-N-CA	5.25	126.64	120.71
1	B	525	GLY	CA-C-N	5.19	131.04	121.70
1	B	525	GLY	C-N-CA	5.19	131.04	121.70
1	B	525	GLY	O-C-N	5.18	127.49	122.41
1	A	388	ALA	N-CA-C	5.11	117.71	110.10
1	A	50	ASP	N-CA-C	5.07	118.95	112.26

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	ASP	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	4068	0	3953	58	0
1	B	4055	0	3939	60	0
2	A	53	0	30	1	0
2	B	53	0	30	5	0
3	A	12	0	11	2	0
3	B	12	0	11	0	0
4	A	19	0	26	3	0
5	A	11	0	18	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	11	0	18	3	0
6	B	21	0	30	0	0
7	A	719	0	0	18	3
7	B	658	0	0	20	2
All	All	9692	0	8066	123	3

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 (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:HIS:NE2	2:B:601:FAD:C8M	1.70	1.54
1:A:33:ASP:OD2	1:A:36:GLU:HG3	1.03	1.19
1:A:33:ASP:OD2	1:A:36:GLU:CG	1.98	1.10
1:A:97:ARG:HH12	1:A:526:LEU:HD21	1.17	1.09
1:B:428:VAL:HB	7:B:1164:HOH:O	0.90	1.06
1:B:48:ASP:CB	7:B:1148:HOH:O	2.06	1.04
1:B:97:ARG:HH22	1:B:526:LEU:HD21	1.18	1.04
1:A:526:LEU:HD22	7:A:1281:HOH:O	1.55	1.02
1:A:97:ARG:HH22	1:A:526:LEU:HD11	1.19	1.02
1:A:526:LEU:HD23	7:A:1141:HOH:O	1.59	1.01
1:A:33:ASP:CG	1:A:36:GLU:HG3	1.87	0.99
1:A:36:GLU:HB3	7:A:1149:HOH:O	1.66	0.93
1:B:526:LEU:HD12	7:B:1056:HOH:O	1.69	0.93
1:B:351:THR:HG21	7:B:928:HOH:O	1.69	0.93
1:B:97:ARG:NH1	1:B:526:LEU:HD11	1.84	0.92
1:A:184:VAL:HG22	1:A:190:VAL:HG12	1.52	0.92
1:A:39:ARG:HH22	5:A:604:P4G:C7	1.85	0.90
1:A:47:GLY:HA2	7:A:776:HOH:O	1.73	0.88
1:B:275:PRO:HG2	1:B:428:VAL:CG2	2.03	0.88
1:A:39:ARG:NH2	5:A:604:P4G:C7	2.37	0.87
1:B:275:PRO:HG2	1:B:428:VAL:HG22	1.56	0.86
1:B:378:GLU:O	1:B:381:LEU:HD13	1.76	0.85
1:B:286:VAL:HG22	1:B:381:LEU:CD1	2.08	0.84
1:B:311:GLU:OE1	7:B:701:HOH:O	1.94	0.84
1:B:193:THR:HG21	1:B:216:ASP:OD1	1.78	0.83
1:A:286:VAL:HG22	1:A:381:LEU:CD1	2.08	0.83
1:B:286:VAL:HG22	1:B:381:LEU:HD11	1.61	0.82
1:A:39:ARG:NH2	5:A:604:P4G:H71	1.94	0.81
1:B:97:ARG:HH12	1:B:526:LEU:HD11	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLN:HG3	7:A:715:HOH:O	1.80	0.80
1:A:39:ARG:NH2	5:A:604:P4G:H72	1.96	0.80
1:A:193:THR:HG21	1:A:216:ASP:OD1	1.80	0.80
1:B:97:ARG:NH2	1:B:526:LEU:HD21	1.96	0.79
1:A:286:VAL:HG22	1:A:381:LEU:HD11	1.66	0.78
1:A:97:ARG:NH2	1:A:526:LEU:HD11	1.98	0.78
1:B:489:ASP:HB3	7:B:904:HOH:O	1.87	0.75
1:A:97:ARG:HH12	1:A:526:LEU:CD2	1.97	0.74
1:B:39:ARG:HH12	5:B:606:P4G:H51	1.51	0.74
1:A:39:ARG:HH22	5:A:604:P4G:H72	1.52	0.72
1:A:378:GLU:O	1:A:381:LEU:HD13	1.89	0.72
4:A:603:P6G:O1	7:A:701:HOH:O	2.06	0.72
5:A:604:P4G:H81	7:A:1297:HOH:O	1.89	0.72
1:A:39:ARG:HH22	5:A:604:P4G:H71	1.53	0.71
1:A:23:ASP:O	7:A:702:HOH:O	2.09	0.71
1:A:97:ARG:NH1	1:A:526:LEU:HD21	2.00	0.70
1:B:390:HIS:CD2	2:B:601:FAD:C8M	2.71	0.69
1:B:390:HIS:NE2	2:B:601:FAD:C8	2.55	0.68
1:A:526:LEU:CD2	7:A:1281:HOH:O	2.26	0.67
1:B:356:HIS:HD2	7:B:1192:HOH:O	1.80	0.65
1:A:286:VAL:HG22	1:A:381:LEU:HD12	1.77	0.65
1:B:339:ASP:HB2	7:B:809:HOH:O	1.98	0.61
1:B:348:ARG:NH2	7:B:702:HOH:O	2.10	0.61
1:A:270:PRO:HG2	1:A:337:ILE:HD11	1.82	0.60
1:A:526:LEU:HD13	7:A:1181:HOH:O	2.02	0.60
1:A:525:GLY:O	1:A:526:LEU:HB2	2.01	0.60
1:B:286:VAL:HG22	1:B:381:LEU:HD12	1.83	0.60
1:B:489:ASP:CB	7:B:904:HOH:O	2.50	0.58
3:A:602:EOL:H6	4:A:603:P6G:O19	2.04	0.57
1:B:275:PRO:CG	1:B:428:VAL:CG2	2.81	0.57
1:B:525:GLY:O	1:B:526:LEU:HB2	2.05	0.57
1:A:184:VAL:HG22	1:A:190:VAL:CG1	2.29	0.56
1:B:390:HIS:CE1	2:B:601:FAD:C8M	2.75	0.56
1:A:355:ARG:HG2	1:A:360:ALA:HB2	1.89	0.55
1:B:281:ILE:CD1	7:B:1109:HOH:O	2.54	0.54
1:B:3:ARG:NH1	1:B:11:ASP:OD1	2.40	0.54
1:B:343:GLN:HG2	7:B:1024:HOH:O	2.07	0.54
1:B:289:GLN:HG3	7:B:932:HOH:O	2.07	0.54
1:B:281:ILE:HD12	7:B:1109:HOH:O	2.08	0.53
1:B:281:ILE:HD12	1:B:422:TYR:O	2.08	0.53
1:B:31:ARG:HG2	1:B:36:GLU:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:CG2	1:A:353:GLU:H	2.21	0.53
1:A:289:GLN:CG	7:A:715:HOH:O	2.48	0.52
1:B:39:ARG:NH1	5:B:606:P4G:H51	2.23	0.52
1:A:6:PRO:HD2	1:A:9[A]:VAL:CG2	2.39	0.51
1:B:6:PRO:HD2	1:B:9:VAL:CG2	2.39	0.51
1:A:351:THR:HG22	1:A:353:GLU:H	1.76	0.51
1:B:289:GLN:NE2	7:B:715:HOH:O	2.43	0.51
1:A:193:THR:CG2	1:A:216:ASP:OD1	2.56	0.50
1:B:307:ARG:HD2	7:B:1100:HOH:O	2.12	0.50
1:B:381:LEU:HD23	1:B:438:LEU:CD2	2.42	0.50
1:B:193:THR:CG2	1:B:216:ASP:OD1	2.55	0.50
1:A:33:ASP:OD1	1:A:36:GLU:OE2	2.29	0.50
1:A:67:GLN:CD	1:A:190:VAL:HG13	2.37	0.49
1:A:176:MET:HE1	4:A:603:P6G:H61	1.94	0.49
1:B:351:THR:CG2	1:B:353:GLU:H	2.26	0.49
1:A:6:PRO:O	1:A:9[A]:VAL:HG22	2.13	0.48
1:A:524:LYS:HE3	7:A:755:HOH:O	2.13	0.47
1:B:526:LEU:N	1:B:526:LEU:HD22	2.30	0.47
1:B:270:PRO:HG2	1:B:337:ILE:HD11	1.96	0.47
2:B:601:FAD:O5B	2:B:601:FAD:H8A	2.14	0.47
1:B:517:TRP:CH2	1:B:526:LEU:HD13	2.50	0.46
1:A:303:GLU:CG	7:A:703:HOH:O	2.63	0.46
2:A:601:FAD:O5B	2:A:601:FAD:H8A	2.16	0.45
1:B:97:ARG:HH12	1:B:526:LEU:CD1	2.21	0.45
1:A:33:ASP:CG	1:A:36:GLU:CG	2.72	0.45
1:B:526:LEU:N	1:B:526:LEU:CD2	2.80	0.44
1:A:120:LEU:HD23	1:B:262:LEU:HD21	1.99	0.44
1:A:526:LEU:N	1:A:526:LEU:HD12	2.32	0.44
1:B:275:PRO:HG2	1:B:428:VAL:HG23	1.95	0.44
1:B:289:GLN:CG	7:B:932:HOH:O	2.64	0.44
1:B:207:ILE:HD12	1:B:208:PRO:HD2	1.99	0.44
1:A:24:VAL:HG21	1:A:68:GLU:HG3	2.00	0.43
1:B:262:LEU:HB3	1:B:263:PRO:HD3	2.00	0.43
1:B:524:LYS:HE3	7:B:794:HOH:O	2.17	0.43
1:A:67:GLN:CG	1:A:190:VAL:HG13	2.49	0.42
1:B:381:LEU:HD23	1:B:438:LEU:HD23	2.00	0.42
1:B:52:HIS:CE1	7:B:1159:HOH:O	2.72	0.42
1:A:151:ASP:OD2	3:A:602:EOL:H7A	2.19	0.42
1:A:307:ARG:NH1	7:A:703:HOH:O	2.18	0.42
1:B:350:GLN:HE21	1:B:355:ARG:HG3	1.85	0.42
1:B:275:PRO:CG	1:B:428:VAL:HG23	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLU:HG2	7:A:703:HOH:O	2.19	0.41
1:B:394:SER:HA	1:B:435:HIS:O	2.19	0.41
1:A:6:PRO:HD2	1:A:9[A]:VAL:HG21	2.02	0.41
1:B:351:THR:HG22	1:B:353:GLU:H	1.86	0.41
1:A:390:HIS:HA	1:A:439:LEU:O	2.21	0.41
1:B:270:PRO:HG2	1:B:337:ILE:CD1	2.50	0.41
1:A:158:VAL:HG22	1:A:230:MET:HB3	2.02	0.40
1:A:297:ASP:HB2	7:A:948:HOH:O	2.20	0.40
1:A:238:PRO:HG2	7:A:904:HOH:O	2.22	0.40
1:A:343:GLN:NE2	7:A:727:HOH:O	2.54	0.40
5:B:606:P4G:H51	7:B:1124:HOH:O	2.21	0.40
1:A:262:LEU:HB3	1:A:263:PRO:HD3	2.03	0.40

All (3) 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)
7:A:828:HOH:O	7:B:1238:HOH:O[5_555]	1.74	0.46
7:A:1040:HOH:O	7:B:702:HOH:O[1_665]	1.78	0.42
7:A:710:HOH:O	7:A:1083:HOH:O[6_554]	1.79	0.41

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	524/554 (95%)	513 (98%)	11 (2%)	0	100	100
1	B	522/554 (94%)	510 (98%)	12 (2%)	0	100	100
All	All	1046/1108 (94%)	1023 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	422/444 (95%)	420 (100%)	2 (0%)	81	61
1	B	420/444 (95%)	415 (99%)	5 (1%)	63	34
All	All	842/888 (95%)	835 (99%)	7 (1%)	73	48

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	LYS
1	A	351	THR
1	B	9	VAL
1	B	307	ARG
1	B	327	PRO
1	B	351	THR
1	B	355	ARG

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	52	HIS
1	A	135	HIS
1	A	289	GLN
1	A	343	GLN
1	A	356	HIS
1	B	41	HIS
1	B	52	HIS
1	B	67	GLN
1	B	89	ASN
1	B	350	GLN
1	B	356	HIS
1	B	444	GLN

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 ⓘ

10 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	$\# Z > 2$
5	P4G	A	604	-	10,10,10	0.66	0	9,9,9	1.30	2 (22%)
4	P6G	A	603	-	18,18,18	0.62	0	17,17,17	0.76	0
2	FAD	B	601	-	58,58,58	0.72	1 (1%)	85,89,89	0.84	3 (3%)
2	FAD	A	601	-	58,58,58	0.71	2 (3%)	85,89,89	0.84	2 (2%)
6	PEG	B	604	-	6,6,6	0.14	0	5,5,5	0.23	0
3	EOL	A	602	-	12,12,12	0.42	0	15,15,15	0.49	0
3	EOL	B	602	-	12,12,12	0.32	0	15,15,15	0.62	0
5	P4G	B	606	-	10,10,10	0.54	0	9,9,9	1.20	1 (11%)
6	PEG	B	605	-	6,6,6	0.28	0	5,5,5	0.24	0
6	PEG	B	603	-	6,6,6	0.25	0	5,5,5	0.15	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
5	P4G	A	604	-	-	4/8/8/8	-
4	P6G	A	603	-	-	7/16/16/16	-
2	FAD	B	601	-	-	3/34/50/50	0/6/6/6
2	FAD	A	601	-	-	4/34/50/50	0/6/6/6
6	PEG	B	604	-	-	2/4/4/4	-
3	EOL	A	602	-	-	1/5/5/5	0/1/1/1
3	EOL	B	602	-	-	2/5/5/5	0/1/1/1
5	P4G	B	606	-	-	4/8/8/8	-
6	PEG	B	605	-	-	4/4/4/4	-
6	PEG	B	603	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C1'-C2'	2.60	1.56	1.52
2	A	601	FAD	PA-O3P	2.12	1.61	1.59
2	A	601	FAD	C8A-N9A	-2.12	1.33	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	604	P4G	C2-O2-C3	2.75	122.70	113.06
5	B	606	P4G	O4-C6-C5	-2.69	98.10	110.35
2	A	601	FAD	C4-N3-C2	-2.41	121.36	125.64
2	B	601	FAD	O3P-P-O1P	-2.28	103.85	110.70
2	A	601	FAD	C1'-C2'-C3'	2.10	115.35	109.66
5	A	604	P4G	C7-O4-C6	2.06	120.28	113.06
2	B	601	FAD	O2P-P-O1P	2.01	121.81	112.44
2	B	601	FAD	C4-N3-C2	-2.01	122.07	125.64

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5'-O5'-P-O2P
4	A	603	P6G	C2-C3-O4-C5
4	A	603	P6G	C11-C12-O13-C14
4	A	603	P6G	O10-C11-C12-O13
4	A	603	P6G	O4-C5-C6-O7
4	A	603	P6G	O16-C17-C18-O19

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Mol	Chain	Res	Type	Atoms
6	B	604	PEG	O1-C1-C2-O2
3	A	602	EOL	C2-C7-C8-C9
3	B	602	EOL	C2-C7-C8-C9
6	B	604	PEG	O2-C3-C4-O4
2	A	601	FAD	O4'-C4'-C5'-O5'
2	A	601	FAD	C3'-C4'-C5'-O5'
2	B	601	FAD	C3'-C4'-C5'-O5'
5	B	606	P4G	C8-C7-O4-C6
5	A	604	P4G	C8-C7-O4-C6
2	A	601	FAD	C4'-C5'-O5'-P
2	B	601	FAD	C4'-C5'-O5'-P
5	B	606	P4G	C5-C6-O4-C7
6	B	605	PEG	O1-C1-C2-O2
4	A	603	P6G	C8-C9-O10-C11
4	A	603	P6G	C15-C14-O13-C12
2	B	601	FAD	O4'-C4'-C5'-O5'
6	B	605	PEG	C4-C3-O2-C2
5	A	604	P4G	C5-C6-O4-C7
5	A	604	P4G	C1-C2-O2-C3
6	B	603	PEG	O2-C3-C4-O4
6	B	605	PEG	C1-C2-O2-C3
5	A	604	P4G	O3-C5-C6-O4
6	B	603	PEG	O1-C1-C2-O2
5	B	606	P4G	O3-C5-C6-O4
6	B	605	PEG	O2-C3-C4-O4
5	B	606	P4G	C1-C2-O2-C3
3	B	602	EOL	C1-C2-C7-C8

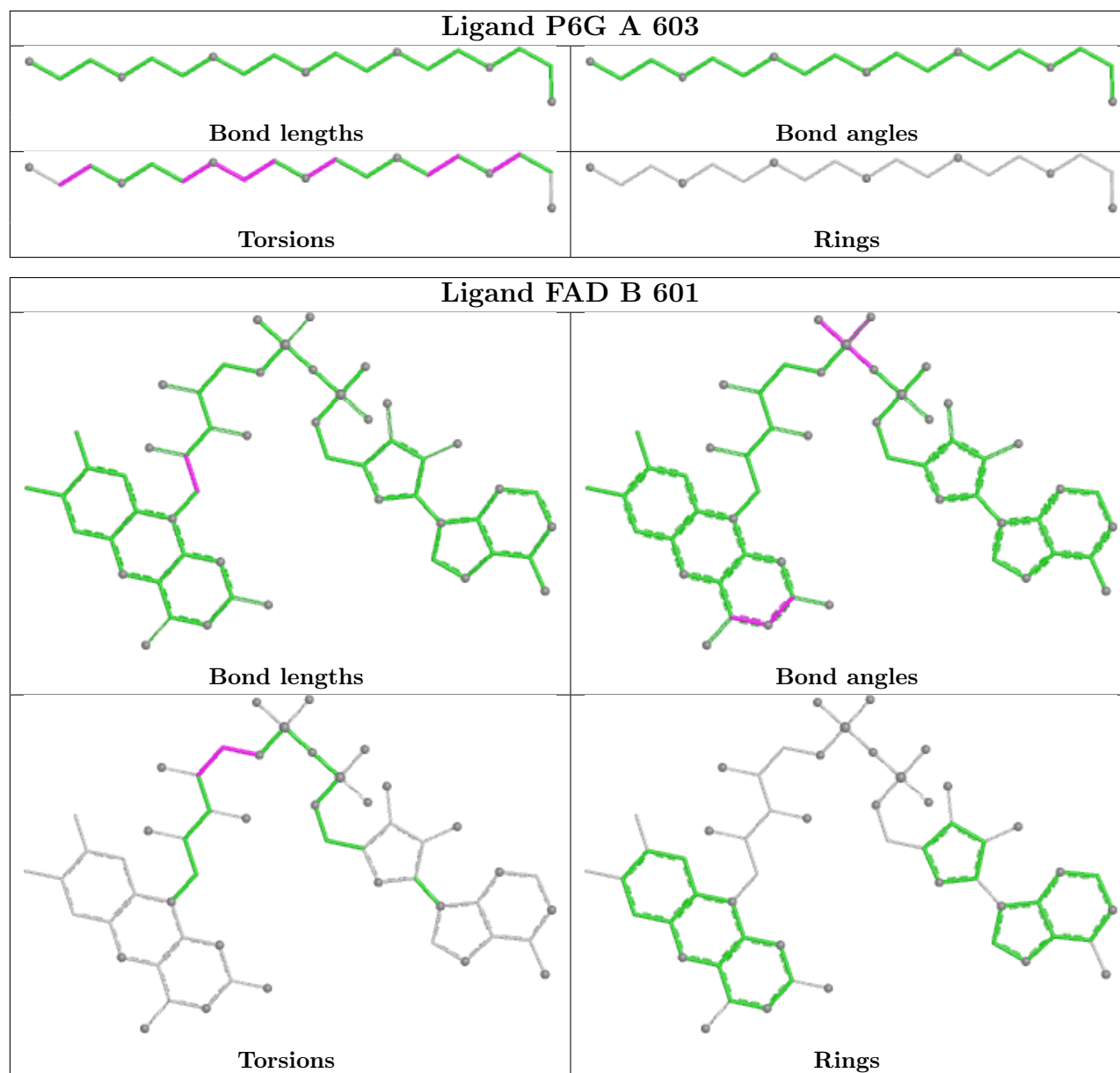
There are no ring outliers.

6 monomers are involved in 20 short contacts:

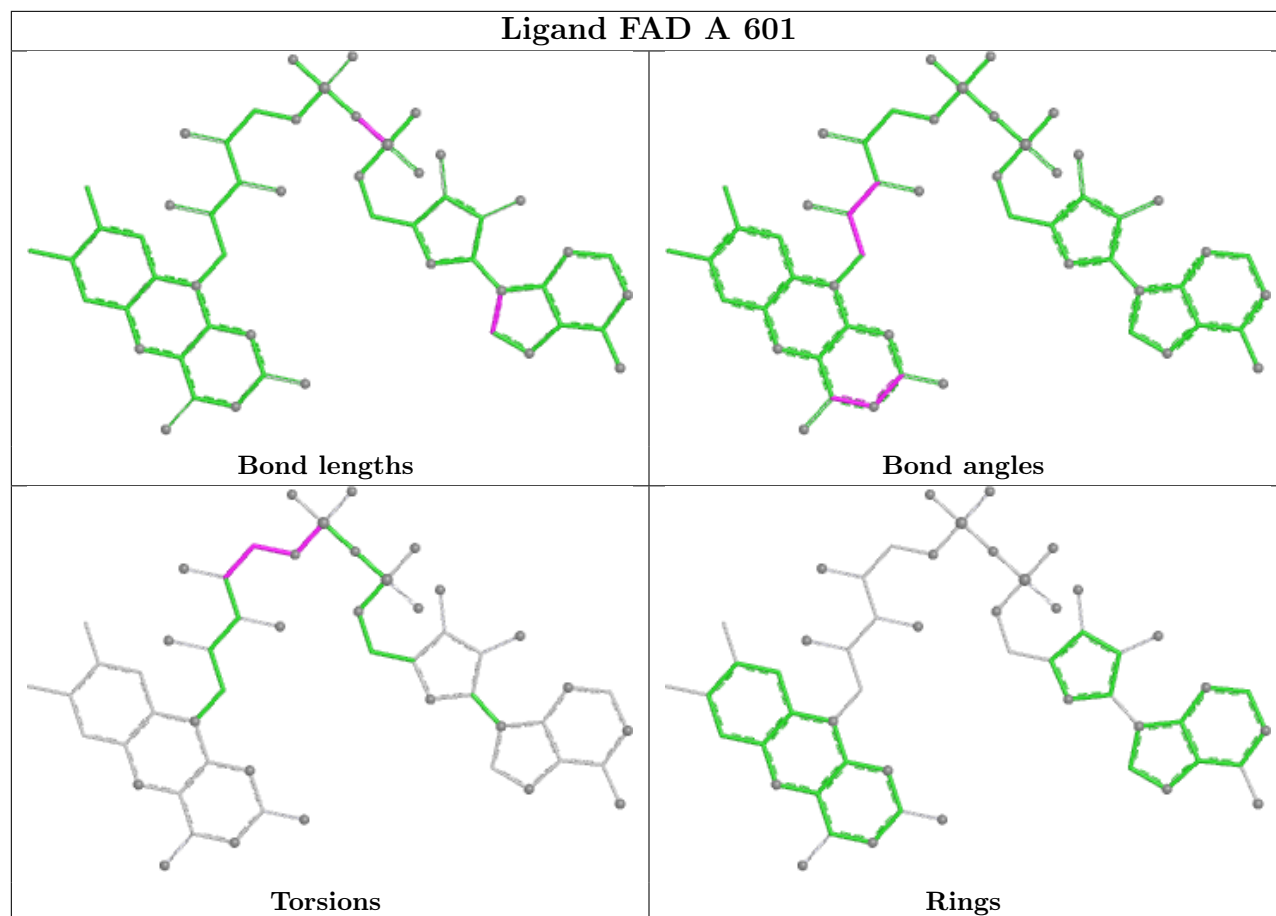
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	P4G	7	0
4	A	603	P6G	3	0
2	B	601	FAD	5	0
2	A	601	FAD	1	0
3	A	602	EOL	2	0
5	B	606	P4G	3	0

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

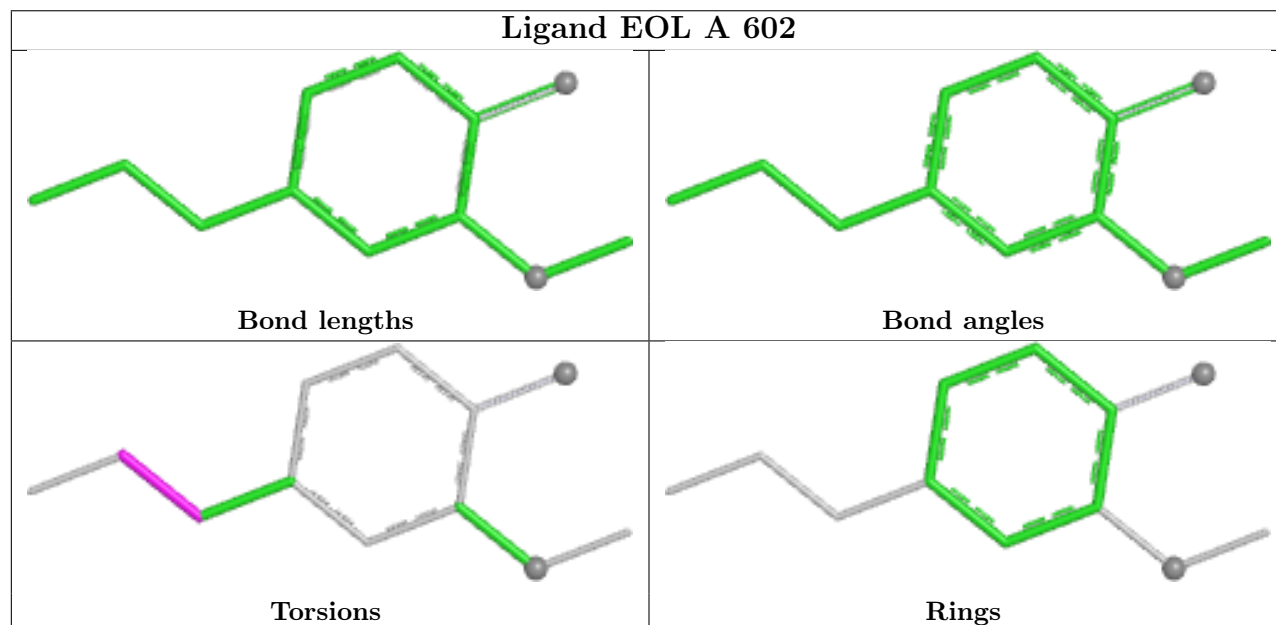
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

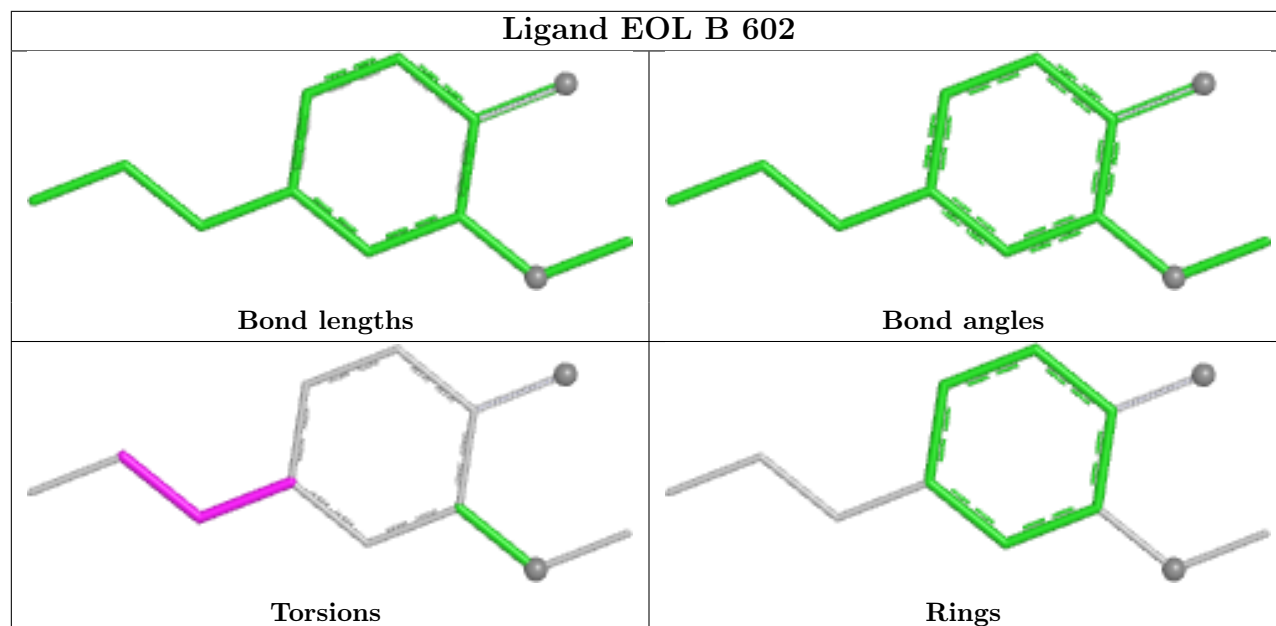


Ligand FAD A 601



Ligand EOL A 602





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	524/554 (94%)	-0.11	13 (2%) 58 61	6, 13, 28, 57	2 (0%)
1	B	524/554 (94%)	0.18	18 (3%) 48 50	9, 17, 32, 53	0
All	All	1048/1108 (94%)	0.03	31 (2%) 52 55	6, 15, 30, 57	2 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	ALA	7.1
1	A	471	TYR	5.2
1	B	526	LEU	4.6
1	A	48	ASP	4.1
1	A	526	LEU	3.9
1	A	51	ALA	3.7
1	A	50	ASP	3.6
1	A	46	VAL	3.5
1	B	471	TYR	3.1
1	A	47	GLY	3.0
1	B	439	LEU	3.0
1	B	49	ALA	2.9
1	A	439	LEU	2.9
1	B	12	GLU	2.9
1	B	50	ASP	2.8
1	B	9	VAL	2.6
1	A	310	LYS	2.6
1	B	295	ASP	2.5
1	A	361	HIS	2.4
1	B	361	HIS	2.4
1	B	15	THR	2.4
1	B	294	TYR	2.3
1	A	249	GLU	2.3
1	B	297	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	343	GLN	2.2
1	B	5	LEU	2.2
1	B	489	ASP	2.1
1	B	438	LEU	2.1
1	B	440	LEU	2.1
1	B	23	ASP	2.1
1	B	337	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

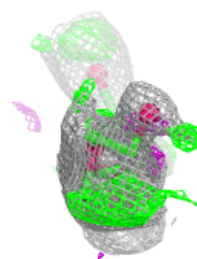
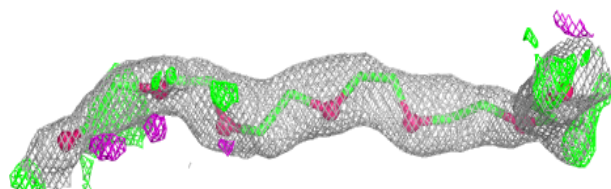
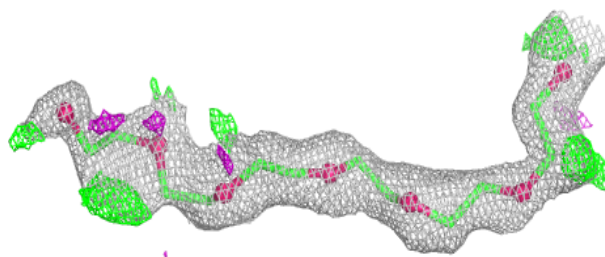
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	P4G	B	606	11/11	0.78	0.17	28,31,37,37	0
4	P6G	A	603	19/19	0.80	0.18	37,40,43,46	0
3	EOL	B	602	12/12	0.80	0.18	34,38,44,50	0
3	EOL	A	602	12/12	0.82	0.15	28,30,38,41	0
5	P4G	A	604	11/11	0.83	0.15	22,23,29,31	0
6	PEG	B	605	7/7	0.84	0.15	36,38,43,48	0
6	PEG	B	603	7/7	0.86	0.15	35,36,37,42	0
6	PEG	B	604	7/7	0.88	0.13	33,34,35,38	0
2	FAD	B	601	53/53	0.98	0.05	11,13,16,18	0
2	FAD	A	601	53/53	0.99	0.04	7,9,12,15	0

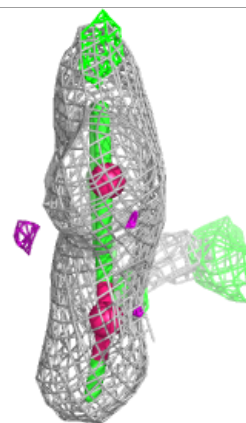
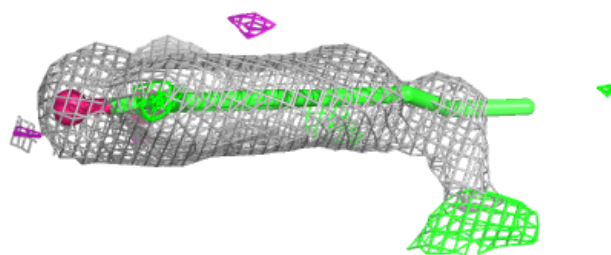
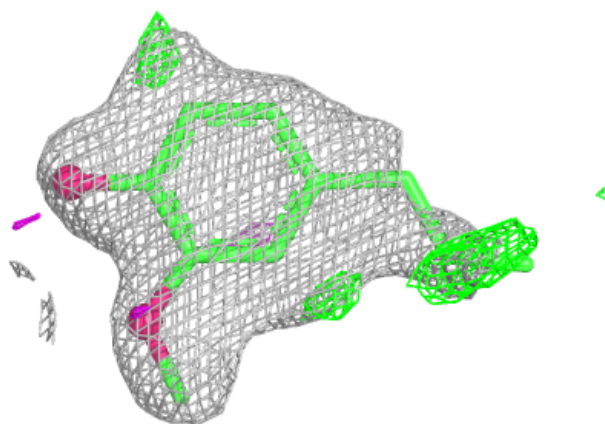
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G A 603:

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

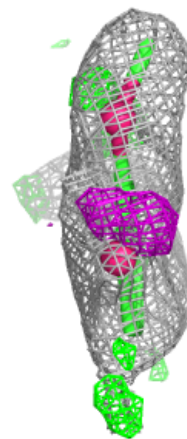
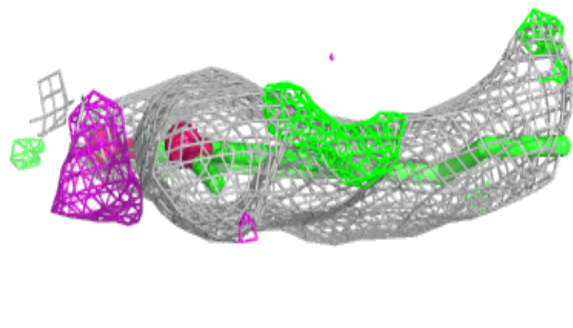
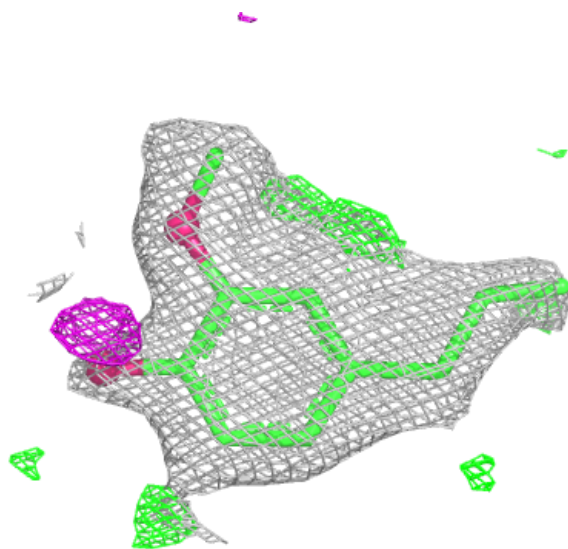
**Electron density around EOL B 602:**

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



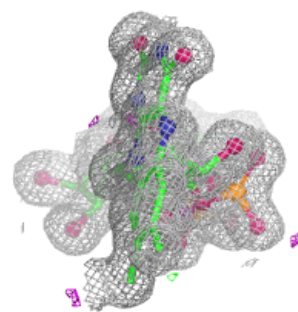
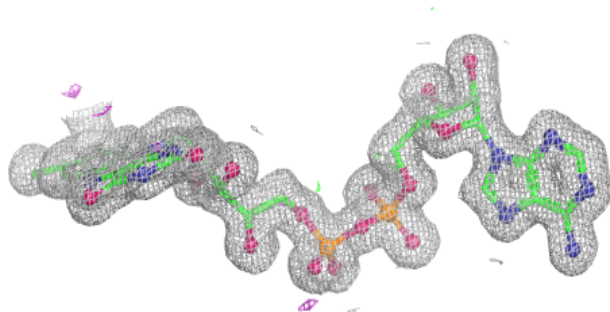
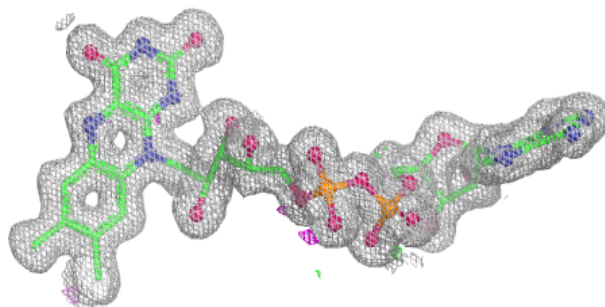
Electron density around EOL A 602:

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

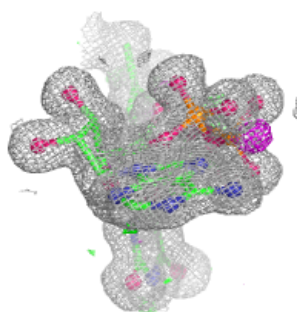
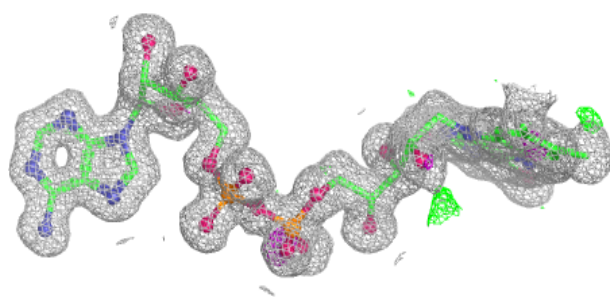
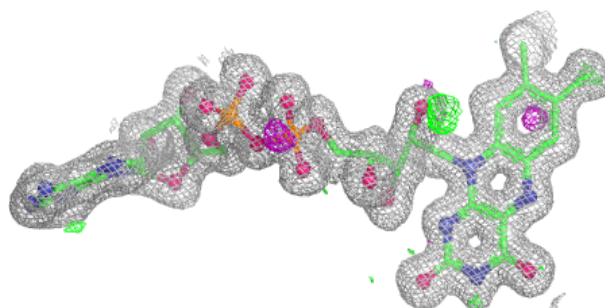


Electron density around FAD B 601:

$2mF_o-DF_c$ (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.