



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 07:17 pm BST

PDB ID : 9FL2
Title : Crystal structure of *Oscillatoria princeps* pyranose oxidase
Authors : Rozeboom, H.J.; Fraaije, M.W.
Deposited on : 2024-06-04
Resolution : 2.64 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

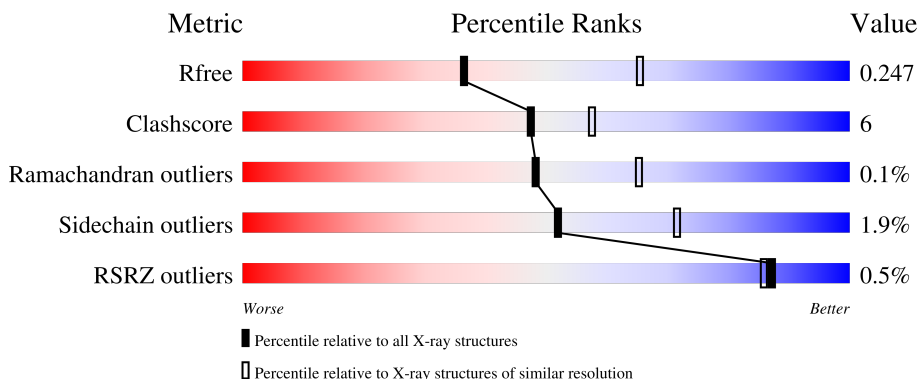
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1851 (2.66-2.62)
Clashscore	180529	1953 (2.66-2.62)
Ramachandran outliers	177936	1929 (2.66-2.62)
Sidechain outliers	177891	1929 (2.66-2.62)
RSRZ outliers	164620	1850 (2.66-2.62)

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	539	82% 14% ..
1	B	539	84% 13% ..
1	C	539	84% 12% ..
1	D	539	85% 12% ..

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 17054 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 pyranose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	526	Total	C	N	O	S	0	0	0
			4186	2671	725	773	17			
1	B	528	Total	C	N	O	S	0	0	0
			4201	2682	728	774	17			
1	C	526	Total	C	N	O	S	0	0	0
			4187	2673	725	772	17			
1	D	527	Total	C	N	O	S	0	0	0
			4191	2676	726	772	17			

- 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	
			Total	C	N	O			P
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		

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

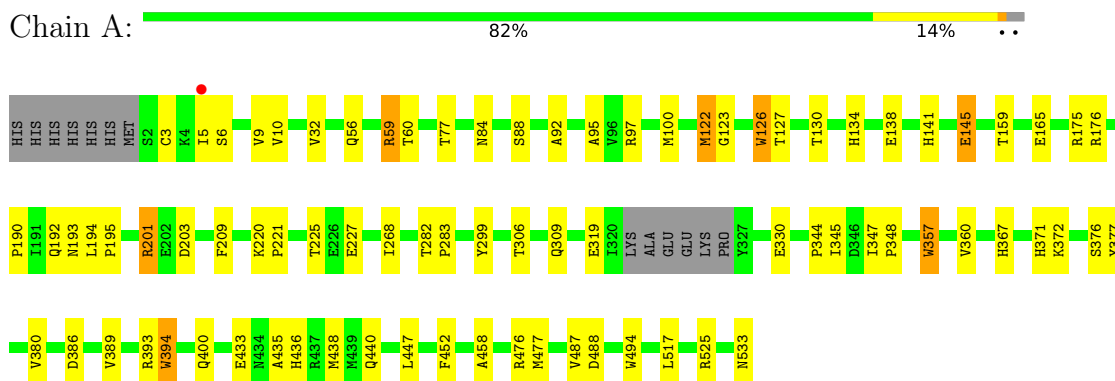
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	22	Total	O	0	0
			22	22		
4	C	15	Total	O	0	0
			15	15		
4	D	20	Total	O	0	0
			20	20		

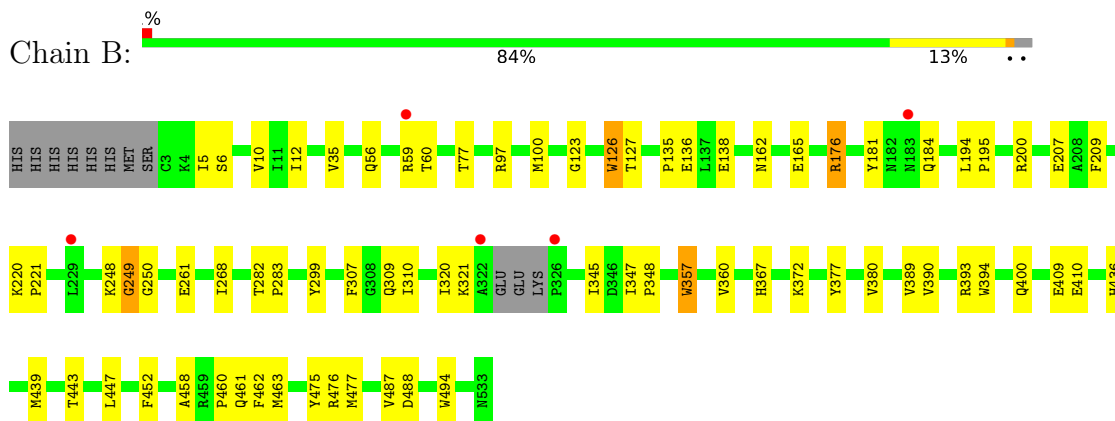
3 Residue-property plots [i](#)

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.

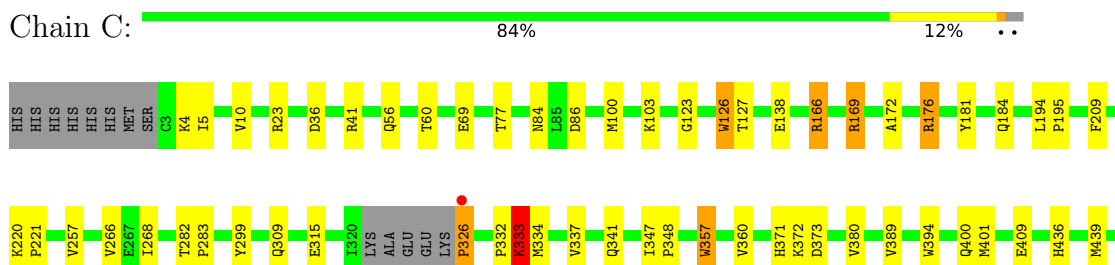
- Molecule 1: pyranose oxidase



- Molecule 1: pyranose oxidase



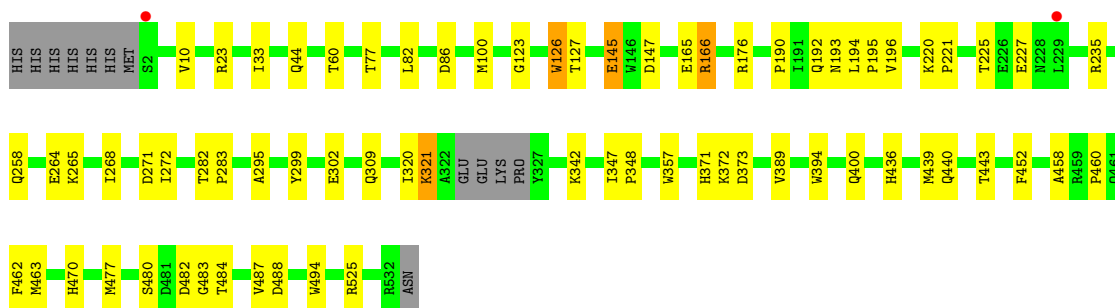
- Molecule 1: pyranose oxidase





- Molecule 1: pyranose oxidase

Chain D: 85% 12% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.97Å 137.41Å 143.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.28 – 2.64 99.28 – 2.64	Depositor EDS
% Data completeness (in resolution range)	61.5 (99.28-2.64) 61.5 (99.28-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.65Å)	Xtrriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.188 , 0.250 0.192 , 0.247	Depositor DCC
R_{free} test set	3054 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtrriage
Anisotropy	0.118	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.010 for -h,l,k	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17054	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.37% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, CL

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	0.41	0/4311	0.87	5/5878 (0.1%)
1	B	0.40	0/4327	0.84	3/5899 (0.1%)
1	C	0.41	0/4313	0.86	5/5881 (0.1%)
1	D	0.40	0/4316	0.83	3/5885 (0.1%)
All	All	0.41	0/17267	0.85	16/23543 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	6
1	D	0	3
All	All	0	14

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	MET	CG-SD-CE	7.36	111.97	100.20
1	A	141	HIS	CB-CA-C	7.00	124.40	110.40
1	A	433	GLU	CB-CA-C	6.43	123.27	110.40
1	C	169	ARG	CB-CA-C	6.33	123.06	110.40
1	C	169	ARG	CG-CD-NE	-6.16	98.86	111.80
1	A	122	MET	CG-SD-CE	-5.60	91.24	100.20
1	A	176	ARG	CA-CB-CG	-5.51	101.28	113.40
1	C	315	GLU	CB-CA-C	5.48	121.36	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	166	ARG	CG-CD-NE	5.39	123.12	111.80
1	A	452	PHE	CB-CA-C	-5.34	99.71	110.40
1	B	176	ARG	CG-CD-NE	-5.23	100.81	111.80
1	C	401	MET	CG-SD-CE	5.16	108.46	100.20
1	B	207	GLU	CB-CA-C	-5.07	100.25	110.40
1	D	463	MET	CG-SD-CE	5.05	108.28	100.20
1	B	452	PHE	CB-CA-C	-5.04	100.31	110.40
1	D	452	PHE	CB-CA-C	-5.02	100.35	110.40

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	ARG	Sidechain
1	A	59	ARG	Sidechain
1	A	97	ARG	Sidechain
1	B	176	ARG	Sidechain
1	B	59	ARG	Sidechain
1	C	166	ARG	Sidechain
1	C	176	ARG	Sidechain
1	C	23	ARG	Sidechain
1	C	326	PRO	Peptide
1	C	333	LYS	Peptide
1	C	532	ARG	Sidechain
1	D	166	ARG	Sidechain
1	D	23	ARG	Sidechain
1	D	483	GLY	Peptide

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	4186	0	4051	52	0
1	B	4201	0	4072	51	0
1	C	4187	0	4054	42	0
1	D	4191	0	4063	51	0
2	A	53	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	30	1	0
2	C	53	0	30	2	0
2	D	53	0	30	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	17	0	0	0	0
4	B	22	0	0	0	0
4	C	15	0	0	1	0
4	D	20	0	0	0	0
All	All	17054	0	16360	184	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 6.

All (184) 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:D:299:TYR:OH	1:D:484:THR:CG2	1.96	1.13
1:D:299:TYR:OH	1:D:484:THR:HG21	1.60	0.99
1:B:307:PHE:HB3	1:B:463:MET:HE3	1.57	0.84
1:A:225:THR:OG1	1:A:227:GLU:HG2	1.77	0.83
1:B:162:ASN:HB2	1:B:165:GLU:OE2	1.82	0.80
1:A:9:VAL:HB	1:A:32:VAL:HG12	1.64	0.79
1:A:175:ARG:NH2	1:A:319:GLU:OE2	2.15	0.79
1:D:225:THR:OG1	1:D:227:GLU:HG2	1.84	0.76
1:D:299:TYR:OH	1:D:484:THR:HG23	1.82	0.76
1:D:299:TYR:HH	1:D:484:THR:HG21	1.53	0.72
1:A:130:THR:HG22	1:A:130:THR:O	1.90	0.71
1:C:181:TYR:O	1:C:184:GLN:HG2	1.90	0.70
1:A:130:THR:HG23	1:A:517:LEU:HD22	1.73	0.69
1:B:181:TYR:O	1:B:184:GLN:HG2	1.92	0.69
1:D:299:TYR:CZ	1:D:484:THR:HG23	2.27	0.69
1:D:194:LEU:C	1:D:194:LEU:HD23	2.14	0.68
1:A:435:ALA:O	1:A:438:MET:HB2	1.94	0.67
1:A:130:THR:HG21	1:A:159:THR:OG1	1.94	0.67
1:D:194:LEU:HD23	1:D:195:PRO:N	2.10	0.67
1:D:295:ALA:HB2	1:D:484:THR:OG1	1.97	0.64
1:A:372:LYS:HE2	1:A:389:VAL:O	1.99	0.63
1:D:44:GLN:HA	1:D:44:GLN:OE1	1.97	0.63
1:C:337:VAL:HG22	1:C:341:GLN:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:LYS:HE2	1:C:389:VAL:O	1.99	0.62
1:C:77:THR:HG21	1:C:100:MET:HB3	1.81	0.61
1:A:77:THR:HG21	1:A:100:MET:HB3	1.82	0.61
1:B:77:THR:HG21	1:B:100:MET:HB3	1.82	0.61
1:D:77:THR:HG21	1:D:100:MET:HB3	1.81	0.61
1:A:130:THR:O	1:A:130:THR:CG2	2.50	0.60
1:A:377:TYR:CE2	1:A:393:ARG:NH1	2.69	0.60
1:D:372:LYS:HE2	1:D:389:VAL:O	2.01	0.60
1:B:377:TYR:CE2	1:B:393:ARG:NH1	2.71	0.59
1:B:12:ILE:HA	1:B:35:VAL:HG23	1.85	0.59
1:B:372:LYS:HE2	1:B:389:VAL:O	2.04	0.58
1:A:145:GLU:OE2	1:A:525:ARG:NH1	2.37	0.57
1:C:4:LYS:C	1:C:5:ILE:HG23	2.24	0.57
1:C:332:PRO:O	1:C:333:LYS:HG2	2.05	0.57
1:D:145:GLU:OE1	1:D:525:ARG:NH1	2.38	0.56
1:C:41:ARG:NH1	1:C:69:GLU:OE2	2.38	0.56
1:D:258:GLN:OE1	1:D:265:LYS:NZ	2.26	0.55
1:B:5:ILE:HG13	1:B:6:SER:H	1.71	0.55
1:D:127:THR:HG23	2:D:601:FAD:H6	1.86	0.54
1:B:248:LYS:O	1:B:249:GLY:C	2.47	0.53
1:B:310:ILE:HD11	1:B:390:VAL:HG22	1.90	0.53
1:D:33:ILE:HD13	1:D:235:ARG:HB3	1.89	0.53
1:C:60:THR:HG21	1:C:380:VAL:HB	1.91	0.53
1:A:447:LEU:O	1:C:436:HIS:NE2	2.38	0.52
1:A:194:LEU:HD12	1:A:195:PRO:HD2	1.92	0.52
1:A:436:HIS:NE2	1:C:447:LEU:O	2.41	0.51
1:B:194:LEU:HD12	1:B:195:PRO:HD2	1.93	0.51
1:B:447:LEU:O	1:D:436:HIS:NE2	2.36	0.51
1:B:12:ILE:HA	1:B:35:VAL:CG2	2.40	0.51
1:B:357:TRP:CE3	1:B:367:HIS:CE1	2.99	0.51
1:D:194:LEU:C	1:D:194:LEU:CD2	2.79	0.51
1:A:440:GLN:HG2	1:C:447:LEU:HB3	1.93	0.50
1:C:257:VAL:CG2	1:C:266:VAL:HB	2.42	0.50
1:A:88:SER:HB3	1:D:436:HIS:HB2	1.93	0.50
1:A:488:ASP:HB3	1:A:494:TRP:CH2	2.47	0.50
1:A:60:THR:HG21	1:A:380:VAL:HB	1.92	0.50
1:A:127:THR:HG23	2:A:601:FAD:H6	1.94	0.49
1:A:357:TRP:CE3	1:A:367:HIS:CE1	3.00	0.49
1:D:194:LEU:HD23	1:D:195:PRO:O	2.14	0.48
1:D:10:VAL:HG21	1:D:268:ILE:HG22	1.95	0.48
1:A:10:VAL:HG21	1:A:268:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ILE:HD11	1:B:390:VAL:CG2	2.43	0.48
1:C:194:LEU:HD12	1:C:195:PRO:HD2	1.94	0.48
1:C:309:GLN:HB2	1:C:458:ALA:HB1	1.96	0.48
1:A:299:TYR:HB3	1:A:400:GLN:HB3	1.97	0.47
1:A:194:LEU:HD13	1:A:357:TRP:HB3	1.95	0.47
1:B:488:ASP:HB3	1:B:494:TRP:CH2	2.49	0.47
1:B:5:ILE:HG13	1:B:6:SER:N	2.29	0.47
1:B:320:ILE:C	1:B:321:LYS:HG2	2.34	0.47
1:B:436:HIS:ND1	1:C:86:ASP:OD2	2.47	0.47
1:B:477:MET:HB3	1:B:487:VAL:HG23	1.96	0.47
1:C:299:TYR:HB3	1:C:400:GLN:HB3	1.96	0.47
1:C:103:LYS:HD2	1:C:409:GLU:OE1	2.14	0.47
1:D:439:MET:HE1	1:D:460:PRO:HB2	1.96	0.47
1:D:347:ILE:O	1:D:348:PRO:C	2.53	0.47
1:B:10:VAL:HG21	1:B:268:ILE:HG22	1.98	0.46
1:B:461:GLN:HG3	1:B:463:MET:HE2	1.98	0.46
1:C:10:VAL:HG21	1:C:268:ILE:HG22	1.97	0.46
1:C:337:VAL:CG2	1:C:341:GLN:O	2.62	0.46
1:D:439:MET:O	1:D:443:THR:HG23	2.14	0.46
1:A:282:THR:HB	1:A:283:PRO:CD	2.45	0.46
1:A:436:HIS:ND1	1:D:86:ASP:OD2	2.48	0.46
1:C:138:GLU:CD	1:C:360:VAL:HG21	2.36	0.46
1:C:347:ILE:O	1:C:348:PRO:C	2.54	0.46
1:D:477:MET:HB3	1:D:487:VAL:HG23	1.98	0.46
1:B:299:TYR:CD2	1:B:476:ARG:HD3	2.50	0.46
1:A:201:ARG:NH1	1:A:203:ASP:OD2	2.49	0.46
1:D:309:GLN:HB2	1:D:458:ALA:HB1	1.98	0.46
1:A:138:GLU:CD	1:A:360:VAL:HG21	2.36	0.46
1:A:309:GLN:HB2	1:A:458:ALA:HB1	1.97	0.46
1:D:82:LEU:CD1	1:D:82:LEU:N	2.79	0.45
1:D:271:ASP:HB2	1:D:272:ILE:HD12	1.98	0.45
1:D:488:ASP:HB3	1:D:494:TRP:CH2	2.51	0.45
1:C:123:GLY:HA2	1:C:126:TRP:CD1	2.52	0.45
1:A:347:ILE:O	1:A:348:PRO:C	2.54	0.45
1:D:282:THR:HB	1:D:283:PRO:CD	2.46	0.45
1:B:127:THR:HG23	2:B:601:FAD:H6	1.97	0.45
1:C:172:ALA:O	1:C:176:ARG:HG2	2.16	0.45
1:B:282:THR:HB	1:B:283:PRO:CD	2.47	0.45
1:B:138:GLU:CD	1:B:360:VAL:HG21	2.37	0.45
1:B:309:GLN:HB2	1:B:458:ALA:HB1	1.98	0.45
1:C:282:THR:HB	1:C:283:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:ASP:HB3	1:C:494:TRP:CH2	2.51	0.45
1:B:283:PRO:HD3	1:B:475:TYR:CD2	2.52	0.45
1:D:299:TYR:HB3	1:D:400:GLN:HB3	1.99	0.45
1:A:84:ASN:HB2	1:D:462:PHE:O	2.17	0.45
1:B:409:GLU:HA	1:B:409:GLU:OE1	2.16	0.45
1:D:165:GLU:HA	1:D:193:ASN:HD21	1.82	0.45
1:B:299:TYR:HB3	1:B:400:GLN:HB3	1.98	0.44
1:B:447:LEU:HB3	1:D:440:GLN:HG2	1.98	0.44
1:C:477:MET:HA	1:C:487:VAL:O	2.17	0.44
4:C:710:HOH:O	1:D:100:MET:CE	2.65	0.44
1:C:4:LYS:O	1:C:5:ILE:HG23	2.18	0.44
1:C:439:MET:O	1:C:443:THR:HG23	2.17	0.44
1:D:123:GLY:HA2	1:D:126:TRP:CD1	2.52	0.44
1:A:5:ILE:HG13	1:A:6:SER:H	1.83	0.44
1:A:123:GLY:HA2	1:A:126:TRP:CD1	2.52	0.44
1:B:123:GLY:HA2	1:B:126:TRP:CD1	2.53	0.44
1:A:165:GLU:HA	1:A:193:ASN:HD21	1.83	0.44
1:C:477:MET:HB3	1:C:487:VAL:HG23	2.00	0.44
1:B:248:LYS:O	1:B:250:GLY:N	2.51	0.44
1:B:439:MET:HE1	1:B:460:PRO:HB2	1.99	0.44
1:D:194:LEU:HD22	1:D:196:VAL:HG13	2.00	0.44
1:A:477:MET:HB3	1:A:487:VAL:HG23	1.99	0.44
1:B:194:LEU:HD13	1:B:357:TRP:HB3	1.99	0.44
1:B:347:ILE:O	1:B:348:PRO:C	2.54	0.44
1:A:5:ILE:HG13	1:A:6:SER:N	2.32	0.43
1:B:60:THR:HG21	1:B:380:VAL:O	2.18	0.43
1:C:36:ASP:OD1	2:C:601:FAD:O2B	2.33	0.43
1:D:220:LYS:N	1:D:221:PRO:CD	2.82	0.43
1:B:56:GLN:HB3	1:B:209:PHE:CD1	2.53	0.43
1:B:220:LYS:N	1:B:221:PRO:CD	2.82	0.43
1:C:532:ARG:HH11	1:C:532:ARG:HB3	1.83	0.43
1:B:5:ILE:CG1	1:B:6:SER:H	2.31	0.43
1:B:439:MET:O	1:B:443:THR:HG23	2.19	0.43
1:A:477:MET:HA	1:A:487:VAL:O	2.19	0.43
1:A:386:ASP:OD1	1:B:97:ARG:NH1	2.51	0.43
1:B:477:MET:HA	1:B:487:VAL:O	2.19	0.43
1:B:462:PHE:O	1:C:84:ASN:HB2	2.19	0.43
1:C:257:VAL:HG11	1:C:268:ILE:HD12	2.01	0.43
1:A:10:VAL:HG21	1:A:268:ILE:CG2	2.49	0.42
1:D:10:VAL:HG21	1:D:268:ILE:CG2	2.49	0.42
1:A:201:ARG:HH11	1:A:203:ASP:CG	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LYS:N	1:A:221:PRO:CD	2.82	0.42
1:C:127:THR:HG23	2:C:601:FAD:H6	2.00	0.42
1:D:320:ILE:O	1:D:321:LYS:HD3	2.19	0.42
1:B:135:PRO:HB2	1:B:136:GLU:OE1	2.19	0.42
1:B:282:THR:HB	1:B:475:TYR:CE2	2.54	0.42
1:C:194:LEU:HD13	1:C:357:TRP:HB3	2.00	0.42
1:A:122:MET:HB2	2:A:601:FAD:O4'	2.19	0.42
1:C:220:LYS:N	1:C:221:PRO:CD	2.83	0.42
1:A:299:TYR:CD2	1:A:476:ARG:HD3	2.54	0.42
1:D:220:LYS:HB3	1:D:221:PRO:HD3	2.01	0.42
1:B:310:ILE:CD1	1:B:390:VAL:HG22	2.49	0.42
1:D:225:THR:OG1	1:D:227:GLU:CG	2.63	0.42
1:A:56:GLN:HB3	1:A:209:PHE:CD1	2.55	0.42
1:D:299:TYR:CE1	1:D:484:THR:HG23	2.53	0.42
1:D:194:LEU:CD2	1:D:195:PRO:O	2.68	0.41
1:C:56:GLN:HB3	1:C:209:PHE:CD1	2.55	0.41
1:D:33:ILE:CD1	1:D:235:ARG:HB3	2.50	0.41
1:A:95:ALA:HB3	1:A:100:MET:HE2	2.03	0.41
1:A:344:PRO:HG2	1:A:345:ILE:HD12	2.02	0.41
1:B:200:ARG:HH21	1:B:200:ARG:HG3	1.85	0.41
1:C:530:ILE:O	1:C:533:ASN:OXT	2.39	0.41
1:C:439:MET:HE1	1:C:460:PRO:HB2	2.02	0.41
1:C:10:VAL:HG21	1:C:268:ILE:CG2	2.51	0.41
1:D:147:ASP:OD1	1:D:147:ASP:O	2.39	0.41
1:D:190:PRO:O	1:D:192:GLN:HG2	2.21	0.41
1:D:477:MET:HA	1:D:487:VAL:O	2.20	0.41
1:A:92:ALA:HB3	1:B:345:ILE:HD13	2.03	0.41
1:C:459:ARG:HB2	1:C:460:PRO:HD2	2.02	0.40
1:A:134:HIS:HB2	1:A:360:VAL:CG2	2.51	0.40
1:A:220:LYS:HB3	1:A:221:PRO:HD3	2.01	0.40
1:C:103:LYS:HD2	1:C:409:GLU:CD	2.41	0.40
1:D:480:SER:C	1:D:482:ASP:H	2.24	0.40
1:A:306:THR:OG1	1:A:394:TRP:HB2	2.21	0.40
1:B:357:TRP:HE3	1:B:367:HIS:CE1	2.40	0.40
1:B:10:VAL:HG21	1:B:268:ILE:CG2	2.50	0.40
1:A:190:PRO:O	1:A:192:GLN:HG2	2.22	0.40
1:A:377:TYR:HE2	1:A:393:ARG:HH11	1.68	0.40
1:D:302:GLU:HA	1:D:470:HIS:O	2.22	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	522/539 (97%)	495 (95%)	26 (5%)	1 (0%)	44	59
1	B	524/539 (97%)	495 (94%)	28 (5%)	1 (0%)	44	59
1	C	522/539 (97%)	495 (95%)	27 (5%)	0	100	100
1	D	523/539 (97%)	496 (95%)	27 (5%)	0	100	100
All	All	2091/2156 (97%)	1981 (95%)	108 (5%)	2 (0%)	48	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	249	GLY
1	A	3	CYS

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	449/461 (97%)	440 (98%)	9 (2%)	50	70
1	B	450/461 (98%)	445 (99%)	5 (1%)	70	83
1	C	449/461 (97%)	439 (98%)	10 (2%)	47	67
1	D	449/461 (97%)	438 (98%)	11 (2%)	44	64
All	All	1797/1844 (98%)	1762 (98%)	35 (2%)	52	71

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

Mol	Chain	Res	Type
1	A	59	ARG
1	A	126	TRP
1	A	145	GLU
1	A	330	GLU
1	A	357	TRP
1	A	371	HIS
1	A	376	SER
1	A	394	TRP
1	A	533	ASN
1	B	126	TRP
1	B	261	GLU
1	B	357	TRP
1	B	394	TRP
1	B	410	GLU
1	C	126	TRP
1	C	166	ARG
1	C	169	ARG
1	C	326	PRO
1	C	333	LYS
1	C	357	TRP
1	C	371	HIS
1	C	373	ASP
1	C	394	TRP
1	C	508	PRO
1	D	60	THR
1	D	126	TRP
1	D	145	GLU
1	D	176	ARG
1	D	264	GLU
1	D	321	LYS
1	D	342	LYS
1	D	357	TRP
1	D	371	HIS
1	D	373	ASP
1	D	394	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	158	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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	D	601	1	53,58,58	0.74	0	68,89,89	1.16	7 (10%)
2	FAD	A	601	1	53,58,58	0.74	1 (1%)	68,89,89	1.11	3 (4%)
2	FAD	C	601	1	53,58,58	0.68	0	68,89,89	0.97	3 (4%)
2	FAD	B	601	1	53,58,58	0.68	0	68,89,89	1.08	5 (7%)

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	D	601	1	-	8/30/50/50	0/6/6/6
2	FAD	A	601	1	-	7/30/50/50	0/6/6/6
2	FAD	C	601	1	-	7/30/50/50	0/6/6/6
2	FAD	B	601	1	-	7/30/50/50	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C1'-C2'	-2.09	1.49	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	O2P-P-O1P	2.90	126.60	112.24
2	A	601	FAD	O2A-PA-O1A	2.77	125.91	112.24
2	D	601	FAD	O2'-C2'-C1'	-2.66	103.37	109.80
2	C	601	FAD	O3B-C3B-C2B	-2.64	103.29	111.82
2	D	601	FAD	O2P-P-O1P	2.55	124.85	112.24
2	B	601	FAD	O2P-P-O1P	2.48	124.49	112.24
2	D	601	FAD	O4B-C1B-C2B	-2.36	103.47	106.93
2	D	601	FAD	O2A-PA-O1A	2.36	123.92	112.24
2	D	601	FAD	C5A-C6A-N6A	2.33	123.90	120.35
2	B	601	FAD	C1'-C2'-C3'	-2.29	103.39	109.79
2	B	601	FAD	O2P-P-O5'	-2.28	97.13	107.75
2	B	601	FAD	P-O3P-PA	2.20	140.38	132.83
2	D	601	FAD	C9-C9A-N10	2.19	124.80	121.84
2	A	601	FAD	C4-C4X-N5	-2.17	115.15	118.23
2	D	601	FAD	O2'-C2'-C3'	2.11	114.23	109.10
2	C	601	FAD	P-O3P-PA	2.04	139.84	132.83
2	C	601	FAD	C5A-C6A-N6A	2.04	123.46	120.35
2	B	601	FAD	C5A-C6A-N6A	2.01	123.40	120.35

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	C5B-O5B-PA-O1A
2	C	601	FAD	C5B-O5B-PA-O2A
2	C	601	FAD	C5B-O5B-PA-O3P
2	C	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	C5B-O5B-PA-O1A
2	D	601	FAD	C5B-O5B-PA-O2A
2	D	601	FAD	C5B-O5B-PA-O3P
2	D	601	FAD	C5'-O5'-P-O2P

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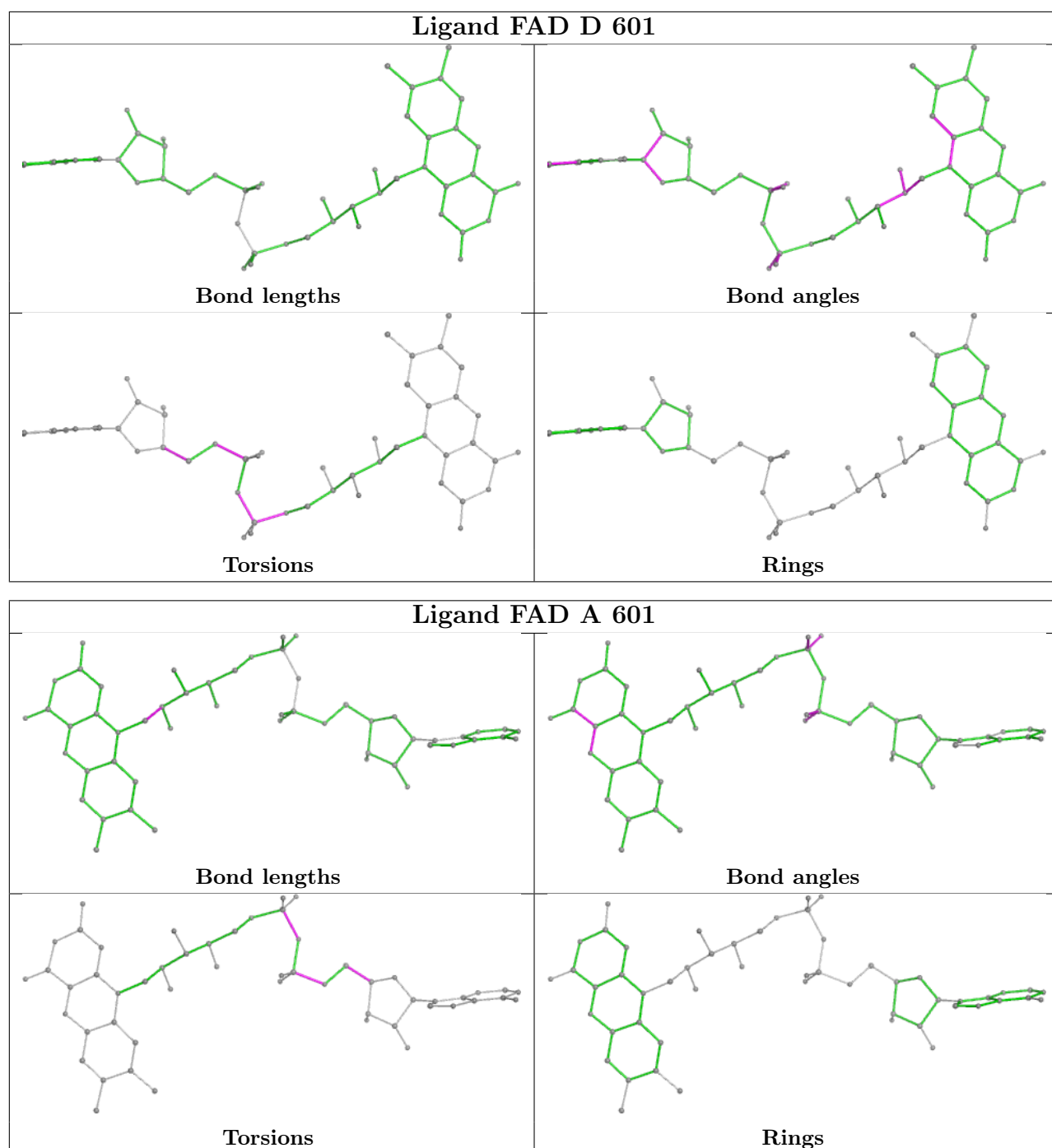
Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C3B-C4B-C5B-O5B
2	C	601	FAD	C3B-C4B-C5B-O5B
2	D	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C3B-C4B-C5B-O5B
2	D	601	FAD	C3B-C4B-C5B-O5B
2	C	601	FAD	PA-O3P-P-O1P
2	A	601	FAD	PA-O3P-P-O5'
2	B	601	FAD	PA-O3P-P-O5'
2	C	601	FAD	PA-O3P-P-O5'
2	D	601	FAD	PA-O3P-P-O5'
2	D	601	FAD	C5'-O5'-P-O3P
2	A	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	PA-O3P-P-O1P
2	B	601	FAD	PA-O3P-P-O1P

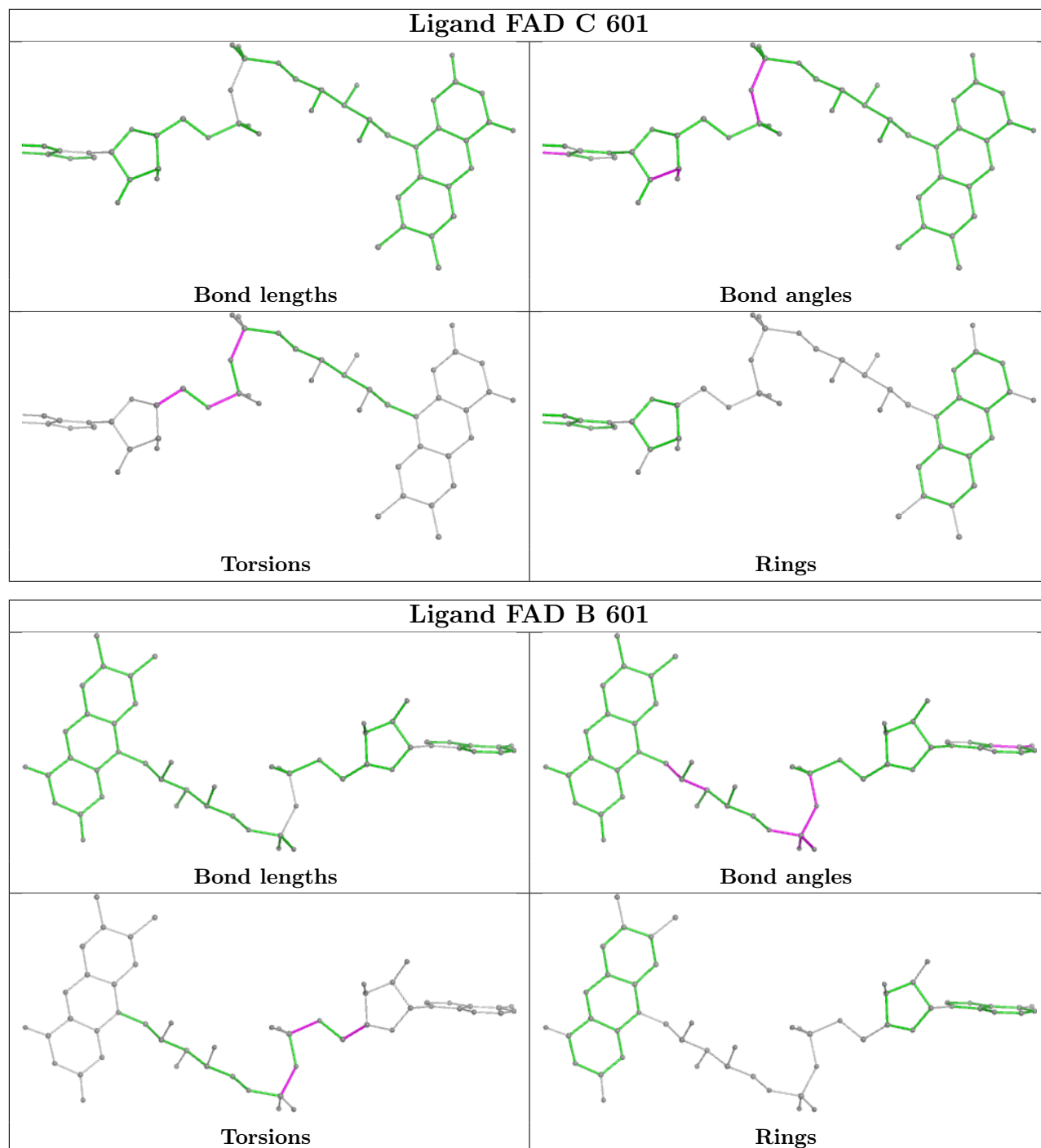
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	FAD	1	0
2	A	601	FAD	2	0
2	C	601	FAD	2	0
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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	526/539 (97%)	-0.41	1 (0%) 92 91	23, 38, 61, 99	0
1	B	528/539 (97%)	-0.33	5 (0%) 81 79	26, 41, 65, 93	0
1	C	526/539 (97%)	-0.34	2 (0%) 89 88	22, 42, 59, 88	0
1	D	527/539 (97%)	-0.40	2 (0%) 89 88	26, 40, 59, 99	0
All	All	2107/2156 (97%)	-0.37	10 (0%) 87 86	22, 40, 61, 99	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	322	ALA	4.5
1	B	326	PRO	2.7
1	B	59	ARG	2.5
1	A	5	ILE	2.3
1	D	229	LEU	2.3
1	D	2	SER	2.2
1	B	183	ASN	2.1
1	C	533	ASN	2.1
1	B	229	LEU	2.1
1	C	326	PRO	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](#)

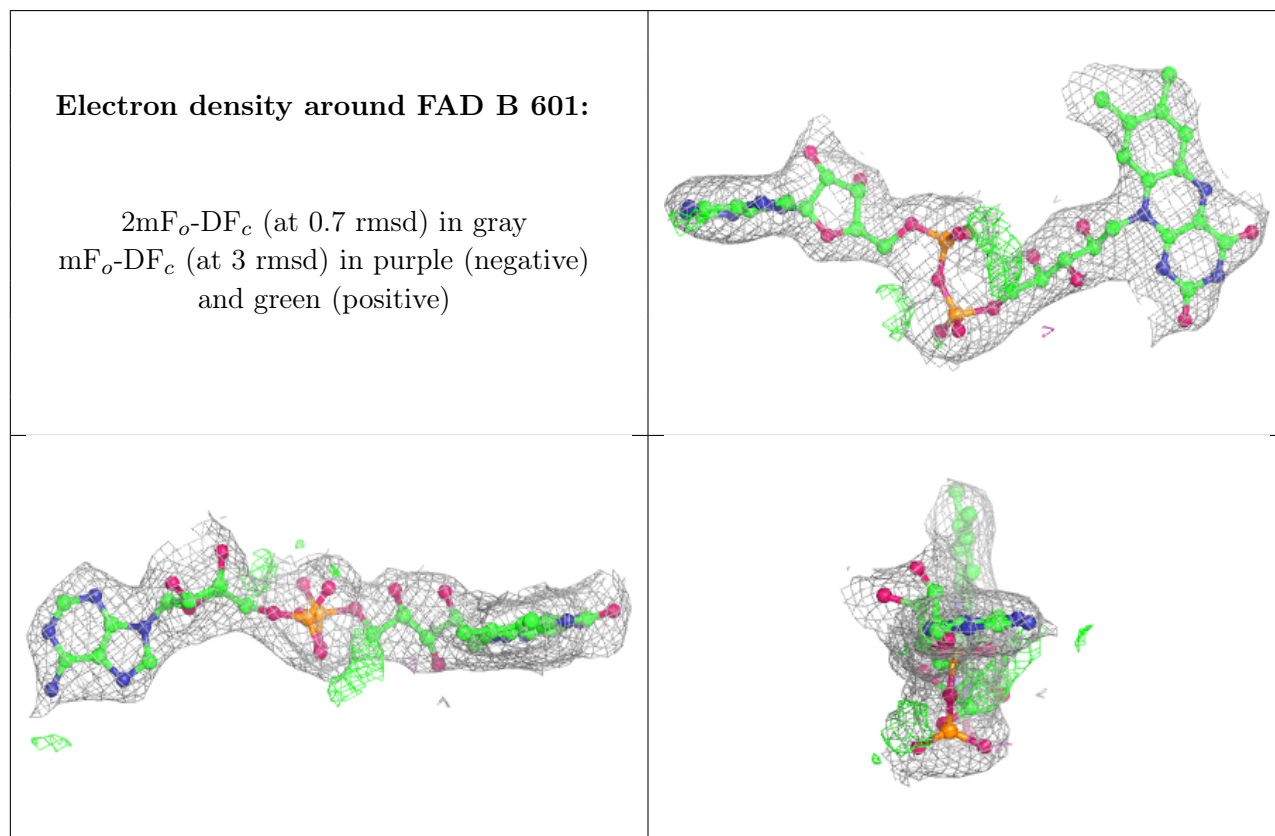
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

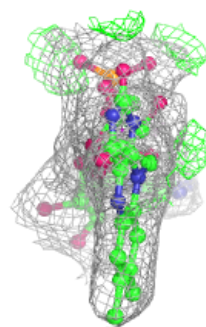
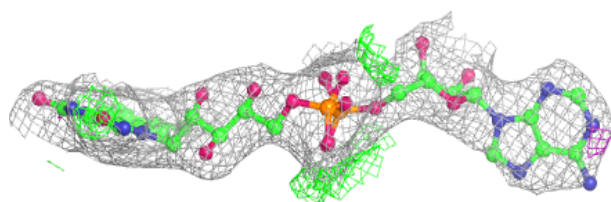
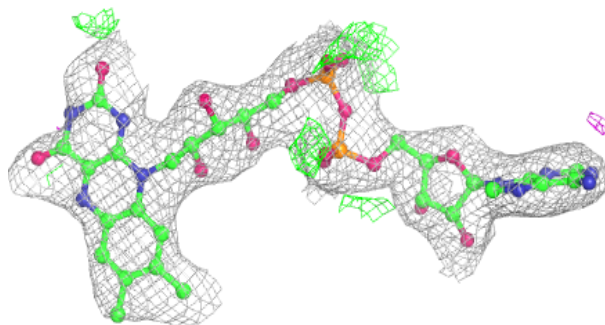
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	B	601	53/53	0.94	0.07	27,34,44,48	0
2	FAD	A	601	53/53	0.95	0.07	28,34,40,44	0
2	FAD	C	601	53/53	0.95	0.07	31,37,47,50	0
2	FAD	D	601	53/53	0.95	0.07	28,32,36,39	0
3	CL	D	602	1/1	0.96	0.13	37,37,37,37	0
3	CL	C	602	1/1	0.97	0.03	31,31,31,31	0
3	CL	B	602	1/1	0.97	0.10	31,31,31,31	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.

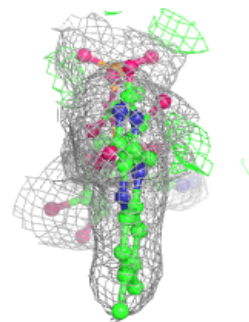
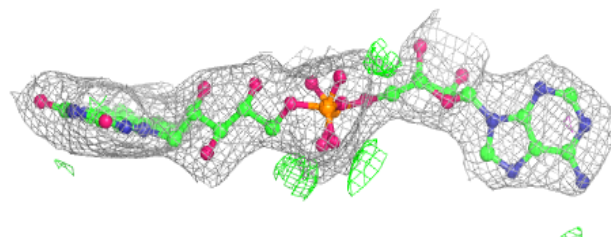
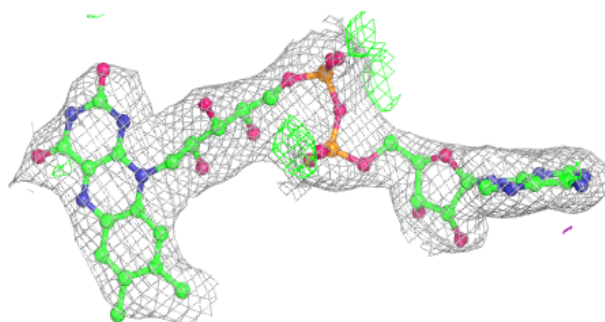


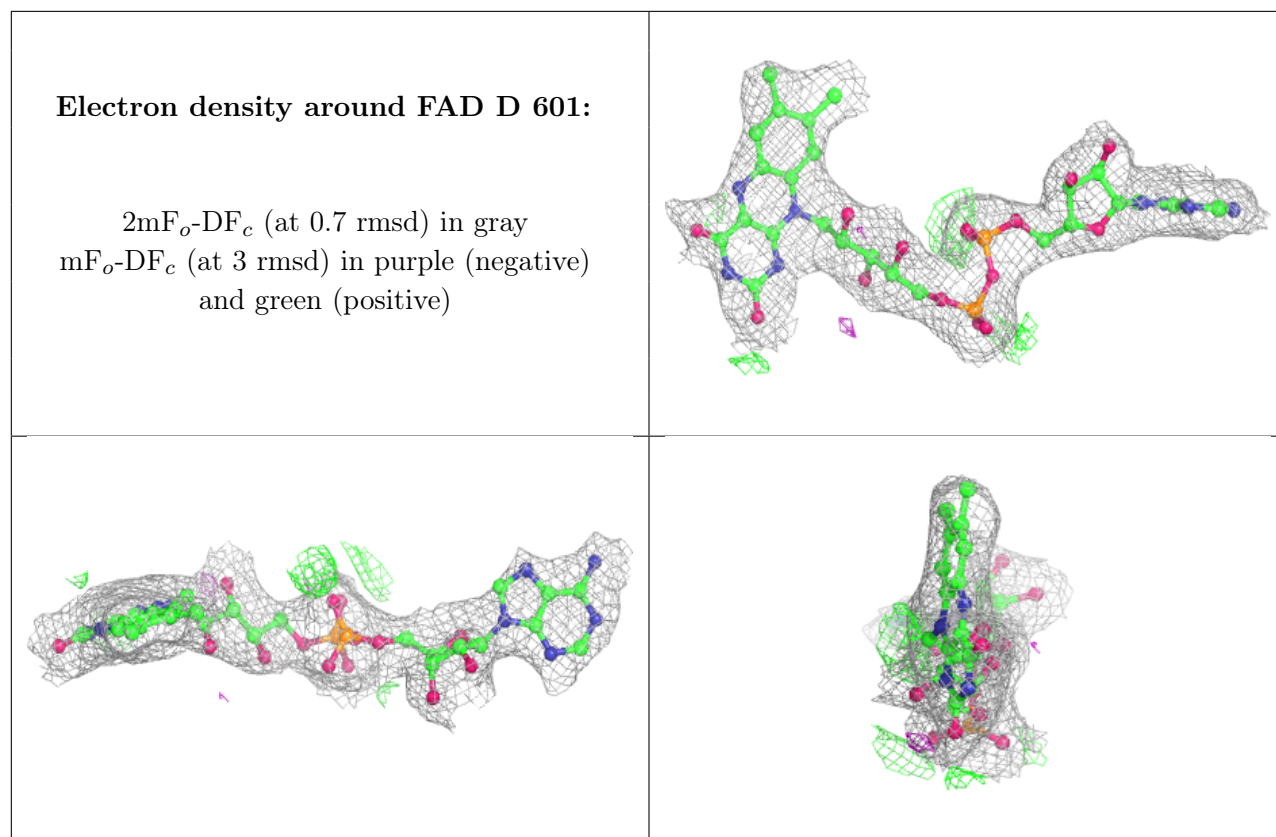
Electron density around FAD A 601:

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

**Electron density around FAD C 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.