



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 02:57 pm GMT

PDB ID : 2IVE  
Title : Structure of protoporphyrinogen oxidase from *Myxococcus xanthus*  
Authors : Corradi, H.R.; Corrigall, A.V.; Boix, E.; Mohan, C.G.; Sturrock, E.D.; Meissner, P.N.; Acharya, K.R.  
Deposited on : 2006-06-13  
Resolution : 2.70 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](mailto: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>.

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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 : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

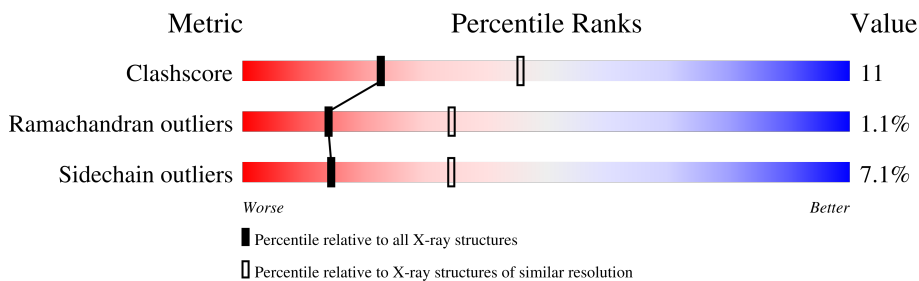
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	478	
1	B	478	

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	TWN	A	4002	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7011 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 PROTOPORPHYRINOGEN OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	451	Total 3326	C 2093	N 627	O 600	S 6	34	0	0
1	B	450	Total 3322	C 2090	N 628	O 598	S 6	29	0	0

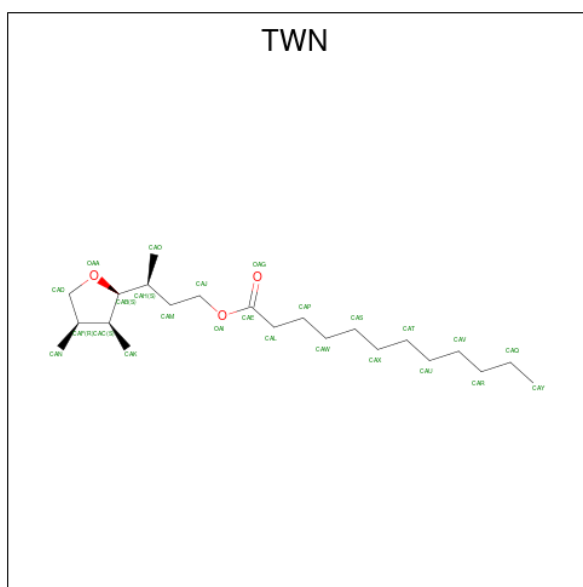
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).





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

- Molecule 4 is (3S)-3-[(2S,3S,4R)-3,4-DIMETHYLTETRAHYDROFURAN-2-YL]BUTYL LAURATE (three-letter code: TWN) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			25	22 3		
4	B	1	Total	C O	0	0
			25	22 3		
4	B	1	Total	C O	0	0
			25	22 3		


- Molecule 5 is water.

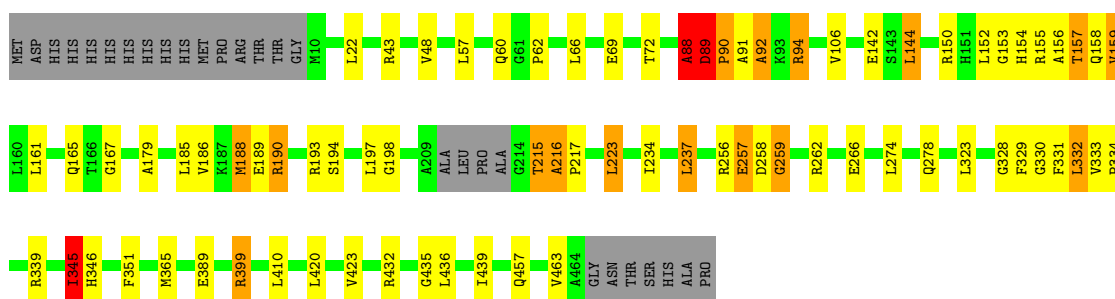
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total	O	0	0
			74	74		
5	B	72	Total	O	0	0
			72	72		

### 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. 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. 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.

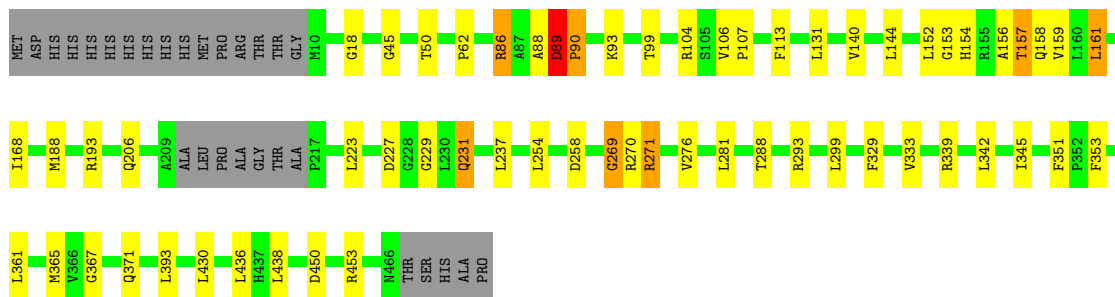
- Molecule 1: PROTOPORPHYRINOGEN OXIDASE

Chain A:  78% 12% •• 6%



- Molecule 1: PROTOPORPHYRINOGEN OXIDASE

Chain B:  81% 11% • 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.57Å 148.57Å 132.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.33 – 2.70 74.28 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (74.33-2.70) 99.9 (74.28-2.70)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.247 , 0.287 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	857 reflections (2.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtrriage
Anisotropy	0.514	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 1.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.52	EDS
Total number of atoms	7011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, TWN, 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	0.37	1/3384 (0.0%)	0.58	2/4593 (0.0%)
1	B	0.37	1/3380 (0.0%)	0.57	3/4586 (0.1%)
All	All	0.37	2/6764 (0.0%)	0.57	5/9179 (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	4
1	B	0	2
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	262	ARG	CD-NE	6.97	1.58	1.46
1	B	93	LYS	CB-CG	-5.40	1.38	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	206	GLN	CG-CD-OE1	-6.10	109.39	121.60
1	A	259	GLY	N-CA-C	-5.56	99.20	113.10
1	B	93	LYS	CA-CB-CG	5.53	125.56	113.40
1	B	89	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	89	ASP	CB-CG-OD2	5.20	122.98	118.30

There are no chirality outliers.



All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	345	ILE	Peptide
1	A	88	ALA	Peptide
1	A	89	ASP	Peptide
1	A	92	ALA	Peptide
1	B	269	GLY	Peptide
1	B	89	ASP	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	3326	0	3382	83	0
1	B	3322	0	3379	53	0
2	A	53	0	31	2	0
2	B	53	0	31	3	0
3	A	18	0	24	2	0
3	B	18	0	24	1	0
4	A	25	0	42	21	0
4	B	50	0	83	17	0
5	A	74	0	0	0	0
5	B	72	0	0	0	0
All	All	7011	0	6996	157	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 11.

All (157) 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:92:ALA:CB	1:A:328:GLY:HA2	1.43	1.45
1:A:92:ALA:HB3	1:A:328:GLY:CA	1.47	1.43
4:B:4003:TWN:HAK3	4:B:4003:TWN:CAO	1.55	1.31
4:B:4003:TWN:HAO1	4:B:4003:TWN:CAK	1.58	1.30
4:A:4002:TWN:HAX2	4:A:4002:TWN:CAR	1.50	1.28
1:B:88:ALA:HB3	1:B:223:LEU:O	1.44	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:HA	1:A:351:PHE:CE2	1.81	1.15
4:A:4002:TWN:HAX2	4:A:4002:TWN:HAR1	1.19	1.15
1:A:89:ASP:HB3	1:A:90:PRO:CD	1.78	1.14
1:B:88:ALA:CB	1:B:351:PHE:HE2	1.60	1.13
1:B:88:ALA:HB2	1:B:351:PHE:HE2	1.00	1.12
4:A:4002:TWN:HAR1	4:A:4002:TWN:CAX	1.79	1.11
1:A:329:PHE:O	1:A:345:ILE:HG23	1.51	1.08
1:B:18:GLY:HA2	1:B:45:GLY:O	1.54	1.07
4:A:4002:TWN:HAX2	4:A:4002:TWN:HAR2	1.32	1.06
1:B:88:ALA:HB2	1:B:351:PHE:CE2	1.91	1.04
1:A:89:ASP:HB3	1:A:90:PRO:HD3	1.04	1.04
1:B:271:ARG:HH11	1:B:271:ARG:CG	1.70	1.04
1:A:190:ARG:HH11	1:A:190:ARG:HG2	1.22	1.03
1:A:345:ILE:HA	1:A:346:HIS:HB2	1.35	1.03
1:A:88:ALA:HB2	1:A:223:LEU:O	1.59	1.03
4:A:4002:TWN:CAR	4:A:4002:TWN:CAX	2.30	1.02
1:B:88:ALA:CB	1:B:351:PHE:CE2	2.42	1.02
4:A:4002:TWN:HAK3	4:A:4002:TWN:HAO1	1.43	1.01
1:A:365:MET:HG3	4:A:4002:TWN:HAJ2	1.42	1.01
1:A:89:ASP:CB	1:A:90:PRO:HD3	1.91	0.99
1:A:92:ALA:CB	1:A:328:GLY:CA	2.18	0.99
1:A:332:LEU:HG	4:A:4002:TWN:HAK2	1.44	0.98
1:B:269:GLY:HA2	1:B:270:ARG:O	1.64	0.98
1:A:88:ALA:CB	1:A:223:LEU:O	2.18	0.92
1:A:167:GLY:O	4:A:4002:TWN:HAW1	1.71	0.91
1:A:92:ALA:HB1	1:A:328:GLY:HA2	1.53	0.91
1:A:88:ALA:HA	1:A:351:PHE:HE2	1.32	0.90
1:B:271:ARG:HH11	1:B:271:ARG:HG3	1.35	0.89
1:A:215:THR:O	1:A:216:ALA:CB	2.19	0.89
1:A:92:ALA:CB	1:A:328:GLY:N	2.37	0.88
1:A:92:ALA:HB3	1:A:328:GLY:N	1.89	0.86
1:A:153:GLY:O	1:A:157:THR:HG22	1.76	0.83
1:A:48:VAL:HB	1:A:234:ILE:HD11	1.60	0.83
1:B:153:GLY:O	1:B:157:THR:HG22	1.80	0.81
1:A:92:ALA:HB3	1:A:328:GLY:HA2	0.82	0.81
1:A:89:ASP:CB	1:A:90:PRO:CD	2.48	0.81
4:B:4001:TWN:OAI	4:B:4001:TWN:HAO2	1.81	0.79
1:A:345:ILE:HG22	1:A:346:HIS:C	2.02	0.79
1:B:88:ALA:CB	1:B:223:LEU:O	2.28	0.79
1:A:88:ALA:CA	1:A:351:PHE:CE2	2.65	0.79
1:B:271:ARG:HG3	1:B:271:ARG:NH1	1.95	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:CA	1:A:351:PHE:HE2	1.97	0.78
1:A:188:MET:CE	1:A:198:GLY:HA3	2.14	0.78
1:B:271:ARG:HH11	1:B:271:ARG:HG2	1.48	0.77
1:A:167:GLY:O	4:A:4002:TWN:CAW	2.33	0.75
1:A:345:ILE:HG22	1:A:346:HIS:O	1.87	0.75
1:A:190:ARG:HG2	1:A:190:ARG:NH1	1.97	0.74
1:A:188:MET:HE3	1:A:198:GLY:HA3	1.69	0.74
1:A:345:ILE:CA	1:A:346:HIS:HB2	2.17	0.74
1:B:86:ARG:HG2	1:B:227:ASP:HA	1.71	0.72
1:B:329:PHE:HE2	4:B:4003:TWN:HAK2	1.55	0.71
1:B:269:GLY:CA	1:B:270:ARG:O	2.36	0.71
1:B:86:ARG:HB3	1:B:353:PHE:CZ	2.26	0.71
1:A:215:THR:O	1:A:216:ALA:HB3	1.91	0.71
1:A:197:LEU:HD11	3:A:3002:GOL:H12	1.72	0.70
1:A:92:ALA:CB	1:A:328:GLY:H	2.07	0.67
1:B:329:PHE:CE2	4:B:4003:TWN:HAK2	2.29	0.67
1:A:193:ARG:HH21	3:A:3002:GOL:H31	1.58	0.66
4:A:4002:TWN:HAR1	4:A:4002:TWN:HAX1	1.73	0.66
1:A:62:PRO:HA	2:A:2114:FAD:N5	2.11	0.66
1:A:92:ALA:HB2	1:A:328:GLY:N	2.10	0.66
1:B:89:ASP:C	1:B:90:PRO:O	2.36	0.63
1:A:43:ARG:NH2	1:A:60:GLN:HE22	1.97	0.63
2:B:2114:FAD:C4X	4:B:4003:TWN:HAT2	2.29	0.63
4:B:4003:TWN:OAG	4:B:4003:TWN:HAO2	1.99	0.62
4:A:4002:TWN:HAK3	4:A:4002:TWN:CAO	2.15	0.62
1:A:215:THR:O	1:A:216:ALA:HB2	2.00	0.62
1:A:150:ARG:NH2	1:A:189:GLU:OE1	2.33	0.61
1:A:88:ALA:HA	1:A:351:PHE:CD2	2.35	0.61
1:B:50:THR:H	1:B:231:GLN:CG	2.12	0.61
4:B:4003:TWN:HAK3	4:B:4003:TWN:HAO1	0.70	0.59
1:B:131:LEU:O	1:B:193:ARG:NH2	2.35	0.59
1:B:50:THR:H	1:B:231:GLN:HG2	1.69	0.58
1:A:278:GLN:HG2	1:A:435:GLY:HA2	1.86	0.57
1:A:399:ARG:HH11	1:A:399:ARG:CG	2.17	0.57
1:B:88:ALA:HB1	1:B:351:PHE:CE2	2.33	0.57
1:B:193:ARG:HH12	3:B:3007:GOL:H12	1.69	0.56
1:A:332:LEU:CG	4:A:4002:TWN:HAK2	2.29	0.55
1:B:168:ILE:HG23	4:B:4003:TWN:HAV2	1.88	0.55
4:B:4003:TWN:CAO	4:B:4003:TWN:CAK	2.30	0.55
1:B:88:ALA:HA	1:B:351:PHE:CD2	2.42	0.55
1:A:48:VAL:HB	1:A:234:ILE:CD1	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:MET:HE1	1:A:198:GLY:HA3	1.88	0.54
2:B:2114:FAD:C4	4:B:4003:TWN:HAT2	2.36	0.54
1:B:62:PRO:HA	2:B:2114:FAD:N5	2.23	0.54
1:A:330:GLY:HA2	1:A:346:HIS:CG	2.44	0.53
1:B:86:ARG:CB	1:B:353:PHE:CZ	2.91	0.53
2:A:2114:FAD:C4X	4:A:4002:TWN:HAS2	2.39	0.52
1:A:332:LEU:HG	4:A:4002:TWN:CAK	2.29	0.51
1:A:92:ALA:HB2	1:A:328:GLY:H	1.71	0.51
1:B:157:THR:HA	1:B:161:LEU:HB2	1.93	0.50
1:B:86:ARG:HG2	1:B:227:ASP:CA	2.40	0.49
1:B:271:ARG:CG	1:B:271:ARG:NH1	2.41	0.49
1:A:345:ILE:HA	1:A:346:HIS:CB	2.22	0.49
1:A:257:GLU:O	1:A:257:GLU:HG3	2.11	0.49
1:A:142:GLU:CD	1:A:150:ARG:HH12	2.16	0.48
1:A:331:PHE:O	4:A:4002:TWN:HAK1	2.13	0.48
4:B:4001:TWN:OAI	4:B:4001:TWN:CAO	2.55	0.48
1:A:420:LEU:O	1:A:423:VAL:HG12	2.13	0.48
1:B:50:THR:H	1:B:231:GLN:HG3	1.78	0.48
1:A:69:GLU:HB3	1:A:72:THR:HG22	1.96	0.48
1:B:86:ARG:O	1:B:88:ALA:N	2.47	0.47
1:A:152:LEU:HB3	1:A:156:ALA:HB3	1.96	0.47
1:B:365:MET:HG3	4:B:4003:TWN:HAJ1	1.96	0.47
1:A:88:ALA:CB	1:A:223:LEU:HB3	2.45	0.47
1:A:88:ALA:O	1:A:89:ASP:O	2.33	0.47
1:A:339:ARG:HD2	1:A:389:GLU:OE1	2.15	0.46
1:A:258:ASP:C	1:A:259:GLY:O	2.50	0.46
1:B:88:ALA:CA	1:B:351:PHE:CE2	2.96	0.46
1:B:50:THR:HG21	1:B:229:GLY:HA3	1.97	0.46
1:A:257:GLU:O	1:A:259:GLY:O	2.34	0.45
1:A:155:ARG:O	1:A:159:VAL:HG13	2.17	0.45
1:B:107:PRO:HG2	1:B:113:PHE:HA	1.98	0.44
1:A:331:PHE:O	4:A:4002:TWN:CAK	2.65	0.44
1:A:399:ARG:CG	1:A:399:ARG:NH1	2.78	0.44
1:B:365:MET:HG3	4:B:4003:TWN:CAJ	2.48	0.44
1:A:167:GLY:O	4:A:4002:TWN:HAW2	2.15	0.44
4:A:4002:TWN:HAO1	4:A:4002:TWN:CAK	2.22	0.44
1:B:86:ARG:HD2	1:B:86:ARG:HA	1.87	0.44
1:A:256:ARG:O	1:A:257:GLU:HB3	2.19	0.43
1:B:89:ASP:O	1:B:90:PRO:O	2.36	0.43
1:B:269:GLY:HA2	1:B:270:ARG:C	2.37	0.43
1:B:367:GLY:O	1:B:371:GLN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLY:O	1:A:346:HIS:HD2	2.02	0.42
4:B:4001:TWN:HAK3	4:B:4001:TWN:CAM	2.49	0.42
1:B:88:ALA:HA	1:B:351:PHE:CE2	2.54	0.42
1:A:144:LEU:HD22	1:A:161:LEU:HD21	2.01	0.42
1:A:345:ILE:CG2	1:A:346:HIS:HB2	2.50	0.42
1:A:329:PHE:CE2	4:A:4002:TWN:HAD1	2.55	0.42
1:B:281:LEU:HD13	1:B:288:THR:HG23	2.02	0.41
1:B:430:LEU:HD11	1:B:438:LEU:HG	2.02	0.41
1:A:92:ALA:HB1	1:A:94:ARG:HB2	2.02	0.41
1:B:86:ARG:HG3	1:B:353:PHE:CE1	2.54	0.41
1:A:154:HIS:O	1:A:158:GLN:HB2	2.21	0.41
1:A:48:VAL:HG22	1:A:62:PRO:HG3	2.01	0.41
1:A:88:ALA:CB	1:A:223:LEU:HD23	2.50	0.41
1:A:399:ARG:NH1	1:A:399:ARG:HG2	2.35	0.41
1:B:86:ARG:HB3	1:B:353:PHE:CE1	2.56	0.41
1:B:99:THR:HG23	1:B:104:ARG:HD2	2.01	0.41
4:B:4003:TWN:HAR1	4:B:4003:TWN:HAT1	1.78	0.41
1:B:345:ILE:CG1	4:B:4003:TWN:HAH	2.50	0.41
1:A:22:LEU:HB3	1:A:237:LEU:HG	2.02	0.41
1:A:179:ALA:HA	1:A:186:VAL:HG21	2.03	0.41
1:A:194:SER:HB3	1:A:197:LEU:HB2	2.03	0.41
1:A:331:PHE:C	4:A:4002:TWN:HAK1	2.40	0.41
1:B:450:ASP:OD1	1:B:453:ARG:NH2	2.53	0.41
1:A:90:PRO:HB2	1:A:91:ALA:H	1.66	0.41
1:A:333:VAL:HA	1:A:334:PRO:HD3	1.93	0.40
1:B:152:LEU:HB3	1:B:156:ALA:HB3	2.03	0.40
1:B:339:ARG:HG3	1:B:393:LEU:HD21	2.03	0.40
1:B:154:HIS:O	1:B:158:GLN:HB2	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	447/478 (94%)	423 (95%)	17 (4%)	7 (2%)	9	24
1	B	446/478 (93%)	426 (96%)	17 (4%)	3 (1%)	22	46
All	All	893/956 (93%)	849 (95%)	34 (4%)	10 (1%)	14	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	A	215	THR
1	A	216	ALA
1	B	89	ASP
1	B	90	PRO
1	B	258	ASP
1	A	90	PRO
1	A	257	GLU
1	A	88	ALA
1	A	217	PRO

### 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	319/344 (93%)	294 (92%)	25 (8%)	12	29
1	B	319/344 (93%)	299 (94%)	20 (6%)	18	40
All	All	638/688 (93%)	593 (93%)	45 (7%)	14	34

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	66	LEU
1	A	94	ARG
1	A	106	VAL
1	A	144	LEU
1	A	157	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	159	VAL
1	A	165	GLN
1	A	185	LEU
1	A	188	MET
1	A	190	ARG
1	A	223	LEU
1	A	237	LEU
1	A	266	GLU
1	A	274	LEU
1	A	323	LEU
1	A	332	LEU
1	A	345	ILE
1	A	399	ARG
1	A	410	LEU
1	A	432	ARG
1	A	436	LEU
1	A	439	ILE
1	A	457	GLN
1	A	463	VAL
1	B	86	ARG
1	B	89	ASP
1	B	106	VAL
1	B	140	VAL
1	B	144	LEU
1	B	157	THR
1	B	159	VAL
1	B	161	LEU
1	B	188	MET
1	B	231	GLN
1	B	237	LEU
1	B	254	LEU
1	B	271	ARG
1	B	276	VAL
1	B	293	ARG
1	B	299	LEU
1	B	333	VAL
1	B	342	LEU
1	B	361	LEU
1	B	436	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	208	GLN
1	A	315	HIS
1	A	346	HIS
1	A	416	ASN
1	A	437	HIS
1	A	457	GLN
1	B	60	GLN
1	B	154	HIS
1	B	457	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	A	3003	-	5,5,5	0.41	0	5,5,5	0.23	0
2	FAD	B	2114	-	53,58,58	1.16	4 (7%)	68,89,89	1.36	10 (14%)
3	GOL	B	3005	-	5,5,5	0.35	0	5,5,5	0.28	0
4	TWN	B	4003	-	25,25,25	0.58	0	25,30,30	1.56	6 (24%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	B	3007	-	5,5,5	0.39	0	5,5,5	0.22	0
4	TWN	A	4002	-	25,25,25	0.63	0	25,30,30	1.16	2 (8%)
3	GOL	A	3001	-	5,5,5	0.33	0	5,5,5	0.36	0
2	FAD	A	2114	-	53,58,58	1.17	4 (7%)	68,89,89	1.38	9 (13%)
3	GOL	A	3002	-	5,5,5	0.37	0	5,5,5	0.21	0
3	GOL	B	3006	-	5,5,5	0.35	0	5,5,5	0.27	0
4	TWN	B	4001	-	25,25,25	0.69	1 (4%)	25,30,30	1.34	6 (24%)

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	GOL	A	3003	-	-	0/4/4/4	-
2	FAD	B	2114	-	-	3/30/50/50	0/6/6/6
3	GOL	B	3005	-	-	3/4/4/4	-
4	TWN	B	4003	-	-	11/21/34/34	0/1/1/1
3	GOL	B	3007	-	-	2/4/4/4	-
4	TWN	A	4002	-	-	12/21/34/34	0/1/1/1
3	GOL	A	3001	-	-	2/4/4/4	-
2	FAD	A	2114	-	-	4/30/50/50	0/6/6/6
3	GOL	A	3002	-	-	2/4/4/4	-
3	GOL	B	3006	-	-	2/4/4/4	-
4	TWN	B	4001	-	-	12/21/34/34	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2114	FAD	C4X-N5	4.26	1.39	1.30
2	B	2114	FAD	C4X-N5	4.18	1.38	1.30
2	A	2114	FAD	C2A-N3A	4.15	1.38	1.32
2	B	2114	FAD	C2A-N3A	4.10	1.38	1.32
2	A	2114	FAD	C10-N1	2.89	1.39	1.33
2	B	2114	FAD	C10-N1	2.83	1.39	1.33
2	B	2114	FAD	C2A-N1A	2.70	1.38	1.33
2	A	2114	FAD	C2A-N1A	2.64	1.38	1.33
4	B	4001	TWN	OAA-CAB	-2.16	1.39	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2114	FAD	N3A-C2A-N1A	-5.57	119.97	128.68
2	B	2114	FAD	N3A-C2A-N1A	-5.57	119.97	128.68
4	B	4003	TWN	OAA-CAB-CAH	3.62	117.27	109.37
4	A	4002	TWN	OAI-CAE-CAL	3.24	122.07	111.91
2	B	2114	FAD	P-O3P-PA	-3.03	122.41	132.83
2	A	2114	FAD	O4-C4-C4X	-3.02	118.59	126.60
2	B	2114	FAD	O4-C4-C4X	-2.97	118.72	126.60
4	B	4003	TWN	OAI-CAE-CAL	2.86	120.89	111.91
2	A	2114	FAD	P-O3P-PA	-2.76	123.34	132.83
2	A	2114	FAD	C4-N3-C2	-2.68	120.69	125.64
4	B	4003	TWN	CAJ-OAI-CAE	-2.66	108.31	116.92
2	B	2114	FAD	C4-N3-C2	-2.64	120.76	125.64
4	B	4001	TWN	OAI-CAE-CAL	2.61	120.11	111.91
2	B	2114	FAD	C4X-C10-N10	2.59	120.26	116.48
4	B	4003	TWN	CAJ-CAM-CAH	-2.57	108.96	114.89
2	A	2114	FAD	C10-C4X-N5	-2.55	119.45	124.86
2	B	2114	FAD	C10-C4X-N5	-2.54	119.46	124.86
2	A	2114	FAD	C9A-C5X-N5	-2.50	119.72	122.43
2	A	2114	FAD	C4X-C4-N3	2.42	119.34	113.19
2	A	2114	FAD	C4X-C10-N10	2.40	119.99	116.48
4	B	4003	TWN	OAI-CAJ-CAM	2.39	113.52	108.16
2	B	2114	FAD	C4X-C4-N3	2.37	119.21	113.19
4	B	4003	TWN	CAD-OAA-CAB	-2.33	103.09	107.84
2	B	2114	FAD	C4X-C10-N1	-2.32	119.35	124.73
4	A	4002	TWN	OAI-CAE-OAG	-2.29	117.81	123.59
2	A	2114	FAD	C4X-C10-N1	-2.28	119.45	124.73
2	B	2114	FAD	C9A-C5X-N5	-2.25	119.99	122.43
4	B	4001	TWN	OAI-CAJ-CAM	2.24	113.19	108.16
4	B	4001	TWN	CAD-OAA-CAB	-2.23	103.28	107.84
4	B	4001	TWN	CAK-CAC-CAF	-2.14	111.13	115.19
4	B	4001	TWN	CAJ-CAM-CAH	-2.10	110.03	114.89
4	B	4001	TWN	CAN-CAF-CAD	-2.04	110.09	113.59
2	B	2114	FAD	C4-C4X-C10	2.01	120.17	116.79

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2114	FAD	N10-C1'-C2'-O2'
2	A	2114	FAD	N10-C1'-C2'-C3'
2	B	2114	FAD	N10-C1'-C2'-O2'

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Mol	Chain	Res	Type	Atoms
3	A	3002	GOL	C1-C2-C3-O3
3	B	3005	GOL	O1-C1-C2-C3
3	B	3006	GOL	C1-C2-C3-O3
3	B	3007	GOL	O1-C1-C2-C3
4	B	4001	TWN	OAG-CAE-OAI-CAJ
4	B	4001	TWN	OAA-CAB-CAH-CAM
4	B	4001	TWN	CAC-CAB-CAH-CAM
4	B	4001	TWN	OAA-CAB-CAH-CAO
4	B	4001	TWN	CAC-CAB-CAH-CAO
4	B	4003	TWN	OAA-CAB-CAH-CAM
4	B	4003	TWN	CAC-CAB-CAH-CAM
4	B	4003	TWN	OAA-CAB-CAH-CAO
4	B	4003	TWN	CAC-CAB-CAH-CAO
4	A	4002	TWN	OAG-CAE-OAI-CAJ
4	A	4002	TWN	CAL-CAE-OAI-CAJ
4	B	4001	TWN	CAL-CAE-OAI-CAJ
4	B	4003	TWN	CAT-CAU-CAV-CAR
4	A	4002	TWN	CAX-CAT-CAU-CAV
4	B	4003	TWN	CAL-CAE-OAI-CAJ
4	B	4003	TWN	OAG-CAE-OAI-CAJ
3	B	3005	GOL	O1-C1-C2-O2
4	B	4001	TWN	OAI-CAJ-CAM-CAH
4	B	4003	TWN	CAL-CAP-CAW-CAS
4	B	4001	TWN	CAQ-CAR-CAV-CAU
4	B	4003	TWN	CAO-CAH-CAM-CAJ
4	B	4001	TWN	CAW-CAS-CAX-CAT
4	B	4003	TWN	CAX-CAS-CAW-CAP
3	A	3001	GOL	C1-C2-C3-O3
3	B	3005	GOL	C1-C2-C3-O3
4	A	4002	TWN	CAX-CAS-CAW-CAP
4	A	4002	TWN	CAL-CAP-CAW-CAS
4	B	4001	TWN	CAL-CAP-CAW-CAS
3	A	3002	GOL	O2-C2-C3-O3
3	B	3007	GOL	O1-C1-C2-O2
4	A	4002	TWN	OAI-CAJ-CAM-CAH
4	A	4002	TWN	CAE-CAL-CAP-CAW
2	A	2114	FAD	O4B-C4B-C5B-O5B
3	B	3006	GOL	O2-C2-C3-O3
4	A	4002	TWN	CAW-CAS-CAX-CAT
4	A	4002	TWN	CAT-CAU-CAV-CAR
4	B	4003	TWN	CAY-CAQ-CAR-CAV
3	A	3001	GOL	O2-C2-C3-O3

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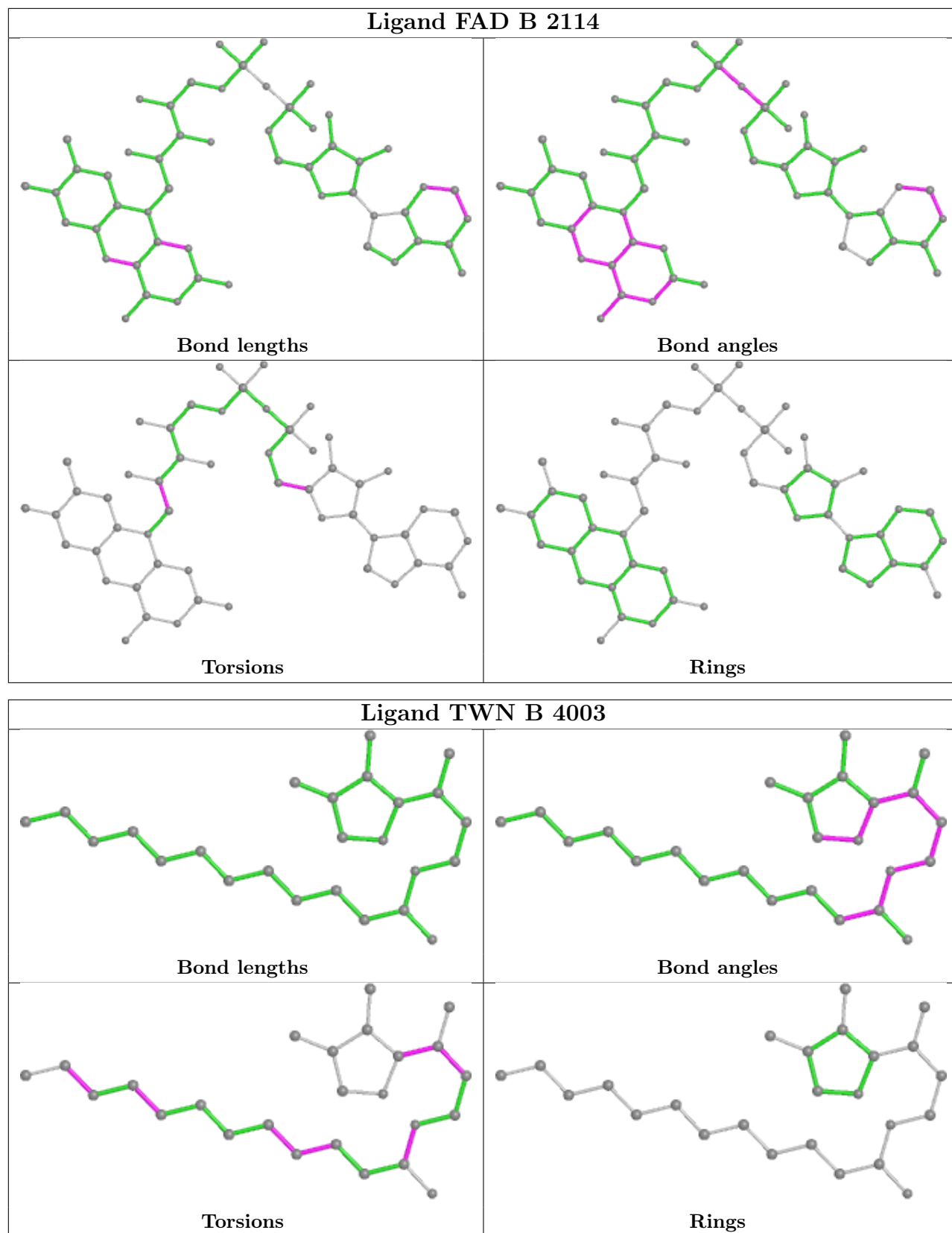
Mol	Chain	Res	Type	Atoms
4	A	4002	TWN	CAU-CAT-CAX-CAS
4	B	4001	TWN	CAT-CAU-CAV-CAR
2	B	2114	FAD	O4B-C4B-C5B-O5B
4	B	4001	TWN	CAX-CAS-CAW-CAP
2	A	2114	FAD	C3B-C4B-C5B-O5B
4	A	4002	TWN	OAI-CAE-CAL-CAP
4	A	4002	TWN	OAG-CAE-CAL-CAP
2	B	2114	FAD	N10-C1'-C2'-C3'

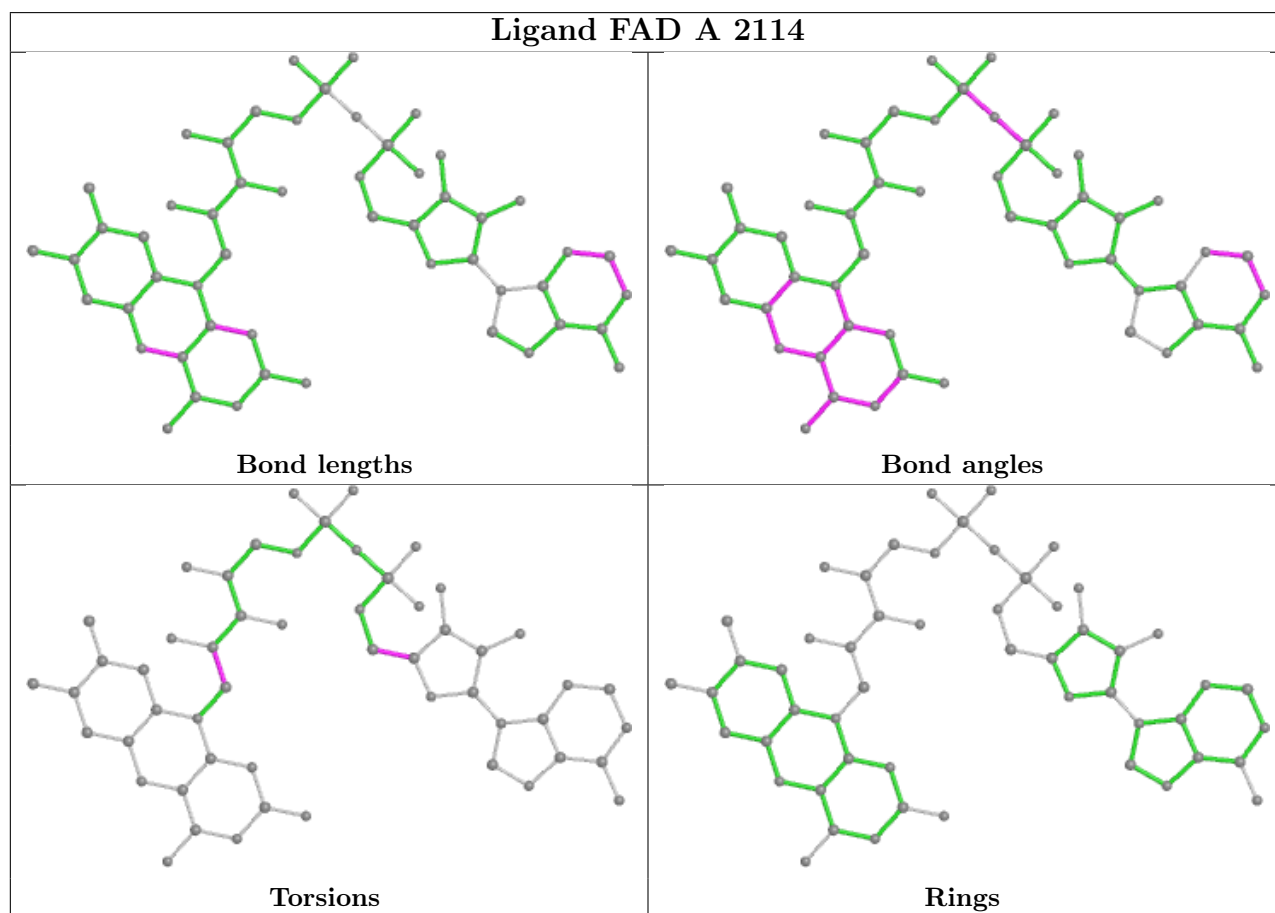
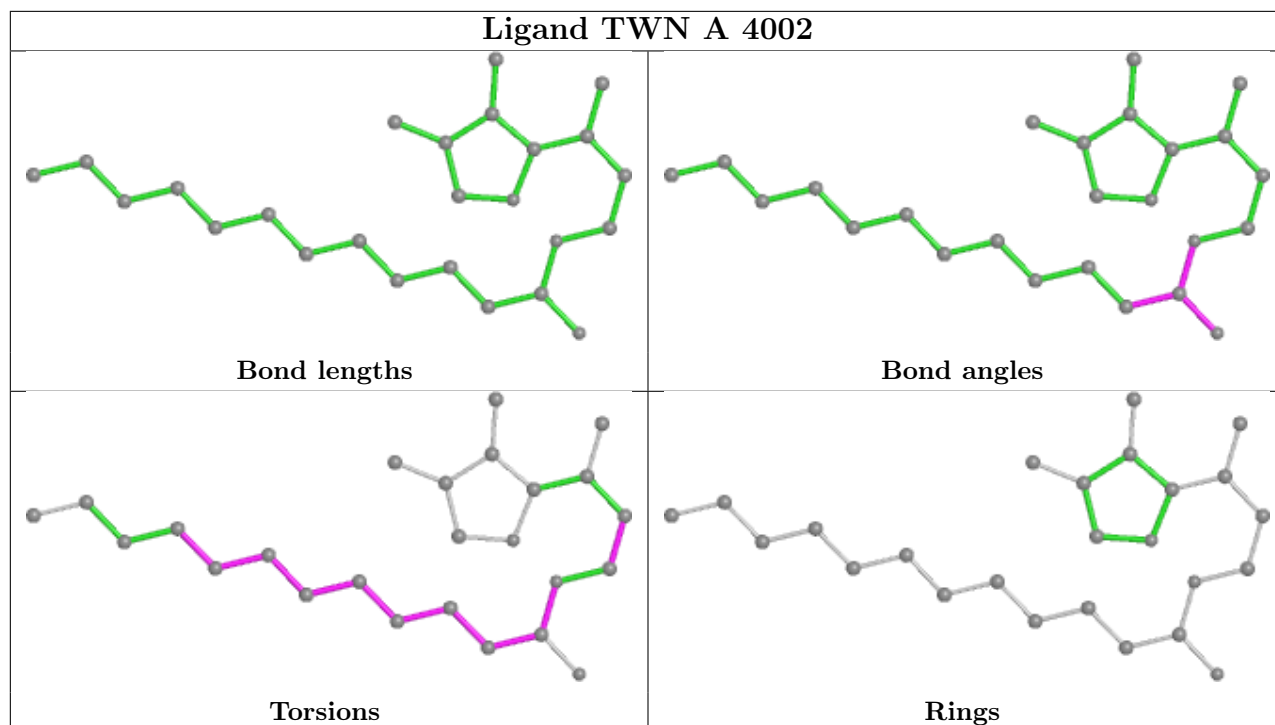
There are no ring outliers.

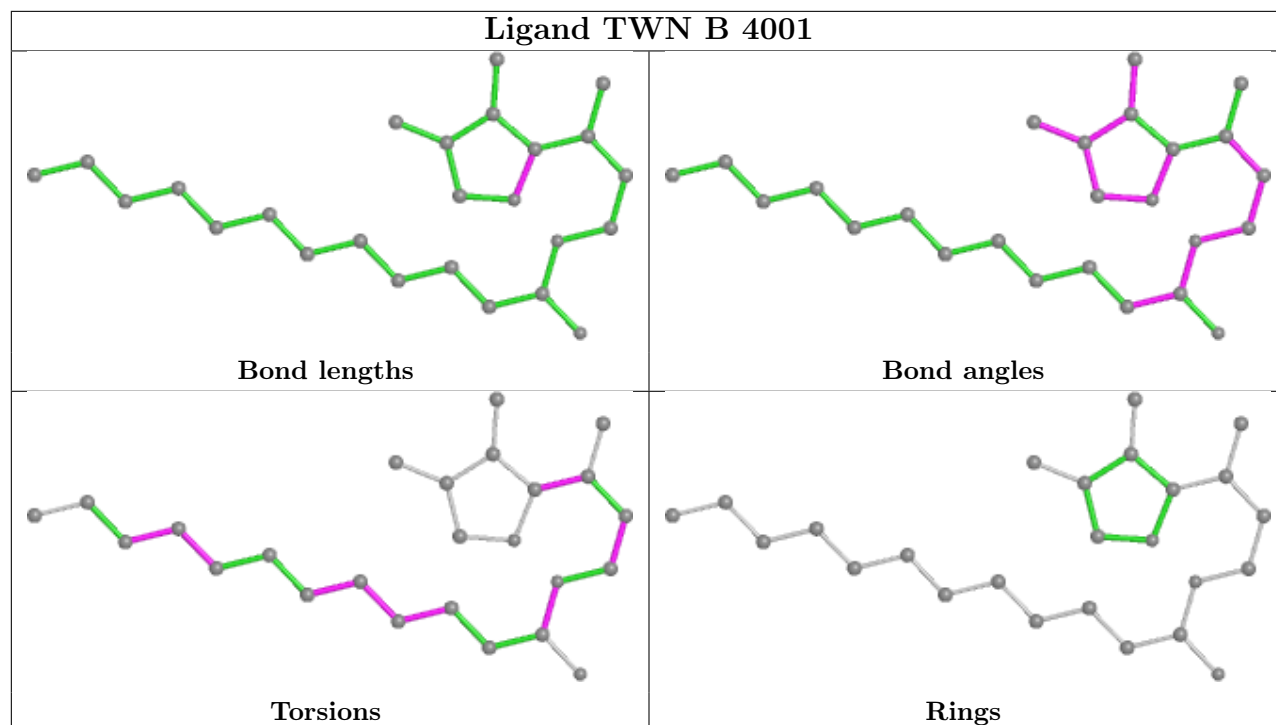
7 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2114	FAD	3	0
4	B	4003	TWN	14	0
3	B	3007	GOL	1	0
4	A	4002	TWN	21	0
2	A	2114	FAD	2	0
3	A	3002	GOL	2	0
4	B	4001	TWN	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.







## 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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

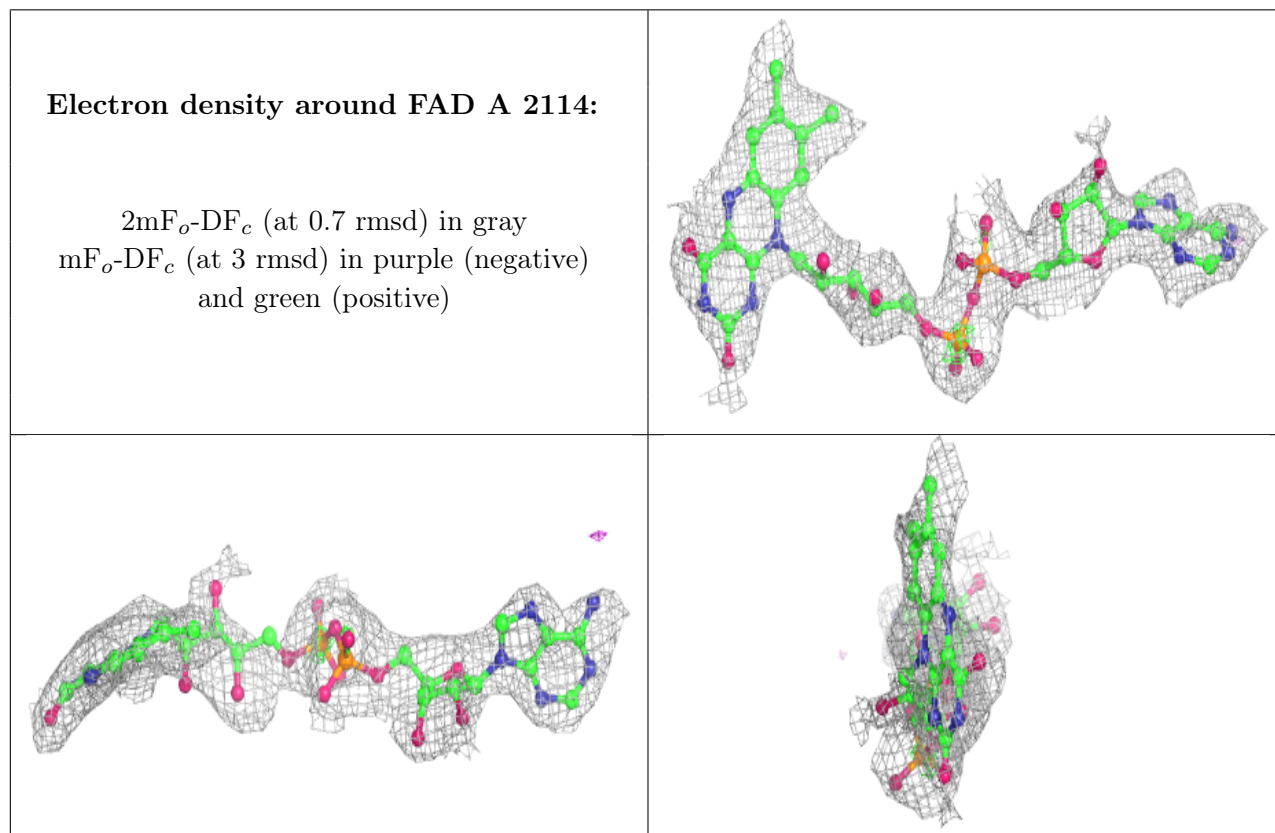
### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

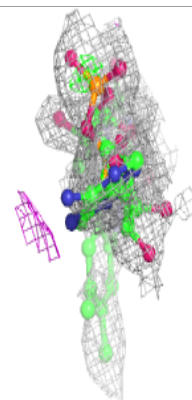
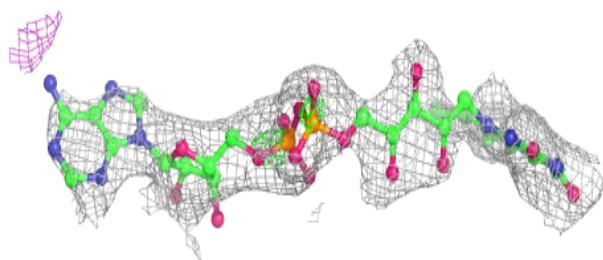
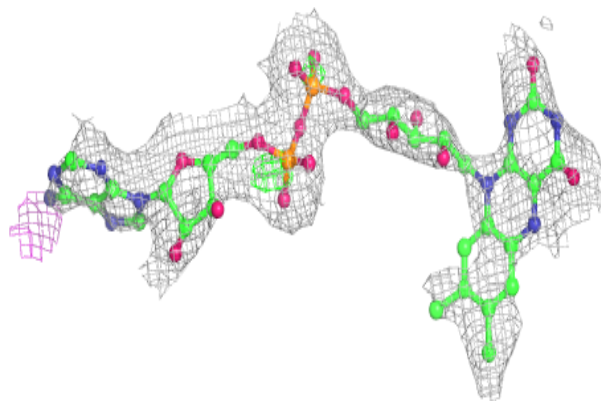
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



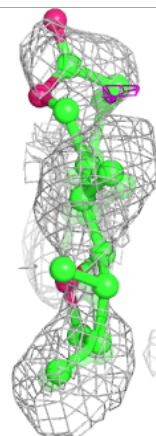
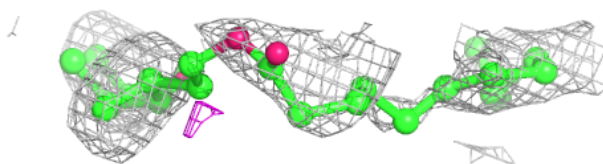
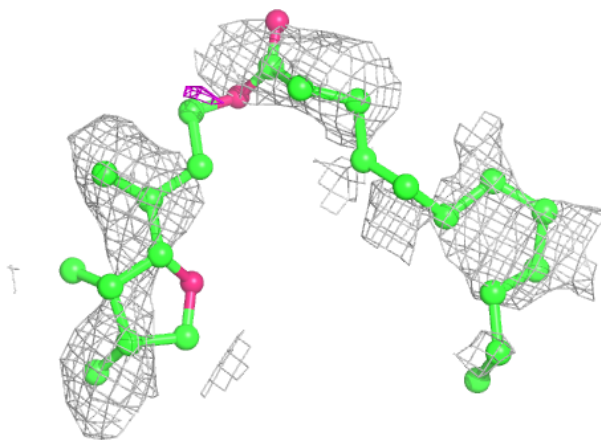


**Electron density around FAD B 2114:**

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

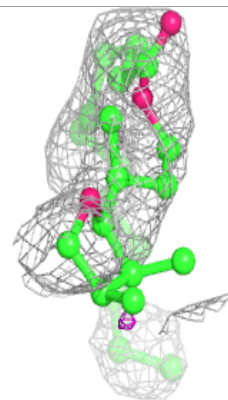
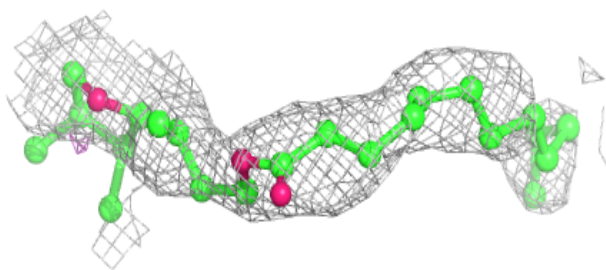
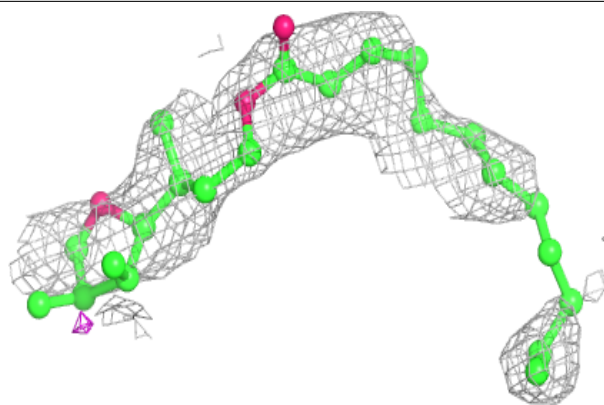
**Electron density around TWN A 4002:**

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

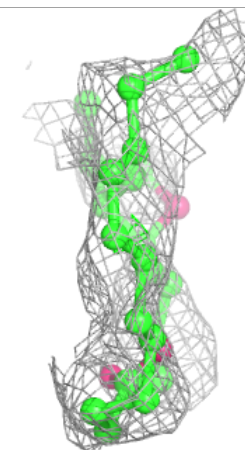
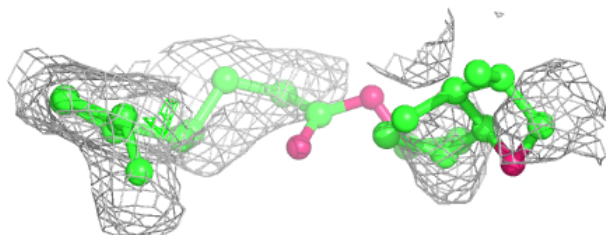
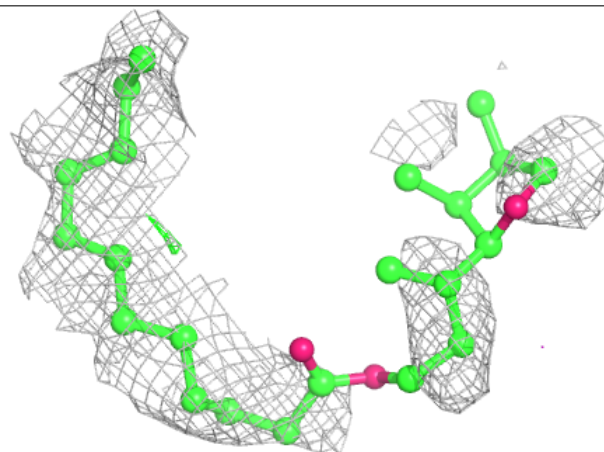


**Electron density around TWN B 4001:**

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

**Electron density around TWN B 4003:**

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



## 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.