



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:36 PM UTC

PDB ID : 4MOL / pdb_00004mol
Title : Pyranose 2-oxidase H167A mutant with 2-fluorinated galactose
Authors : Tan, T.C.; Spadiut, O.; Gandini, R.; Haltrich, D.; Divne, C.
Deposited on : 2013-09-12
Resolution : 2.00 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

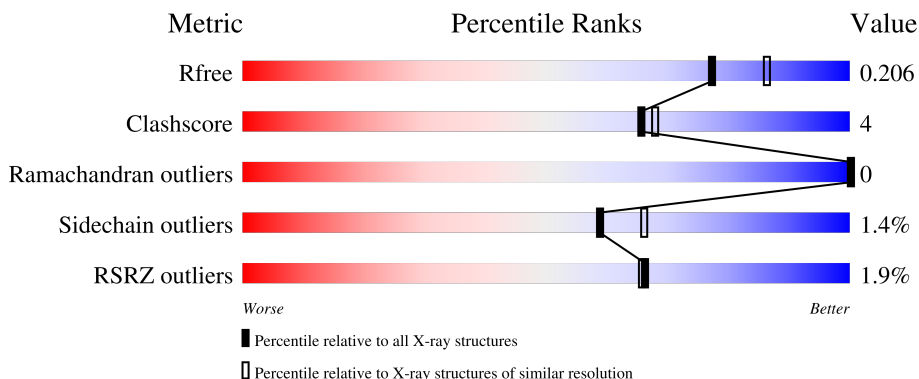
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

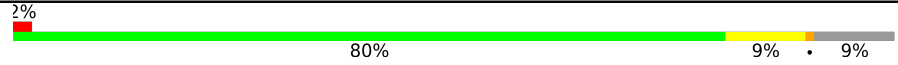



The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	633	 2% 80% 9% • 9%
1	B	633	 3% 83% 8% 9%
1	C	633	 0% 81% 9% • 9%
1	D	633	 0% 82% 8% • 9%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 20233 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 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	573	4535	2863	779	869	24	0	3	0
1	B	576	4545	2870	778	872	25	0	1	0
1	C	573	4521	2855	775	867	24	0	1	0
1	D	573	4521	2855	775	867	24	0	1	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
A	167	ALA	HIS	engineered mutation	UNP Q7ZA32
A	623	ALA	-	expression tag	UNP Q7ZA32
A	624	ALA	-	expression tag	UNP Q7ZA32
A	625	ALA	-	expression tag	UNP Q7ZA32
A	626	LEU	-	expression tag	UNP Q7ZA32
A	627	GLU	-	expression tag	UNP Q7ZA32
A	628	HIS	-	expression tag	UNP Q7ZA32
A	629	HIS	-	expression tag	UNP Q7ZA32
A	630	HIS	-	expression tag	UNP Q7ZA32
A	631	HIS	-	expression tag	UNP Q7ZA32
A	632	HIS	-	expression tag	UNP Q7ZA32
A	633	HIS	-	expression tag	UNP Q7ZA32
B	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
B	167	ALA	HIS	engineered mutation	UNP Q7ZA32
B	623	ALA	-	expression tag	UNP Q7ZA32
B	624	ALA	-	expression tag	UNP Q7ZA32
B	625	ALA	-	expression tag	UNP Q7ZA32
B	626	LEU	-	expression tag	UNP Q7ZA32
B	627	GLU	-	expression tag	UNP Q7ZA32
B	628	HIS	-	expression tag	UNP Q7ZA32

Continued on next page...

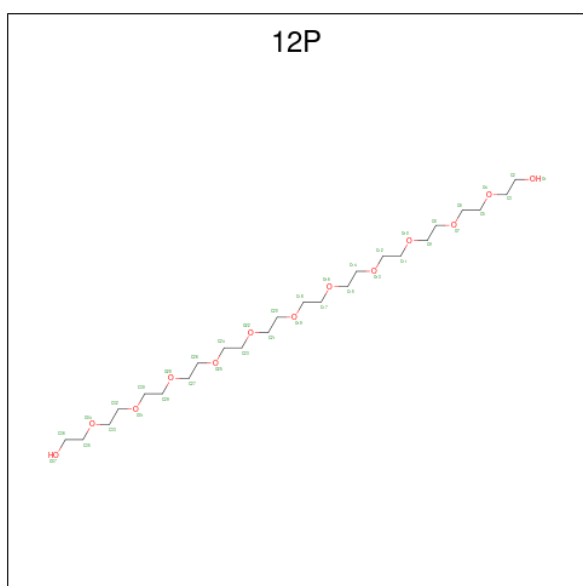
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	629	HIS	-	expression tag	UNP Q7ZA32
B	630	HIS	-	expression tag	UNP Q7ZA32
B	631	HIS	-	expression tag	UNP Q7ZA32
B	632	HIS	-	expression tag	UNP Q7ZA32
B	633	HIS	-	expression tag	UNP Q7ZA32
C	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
C	167	ALA	HIS	engineered mutation	UNP Q7ZA32
C	623	ALA	-	expression tag	UNP Q7ZA32
C	624	ALA	-	expression tag	UNP Q7ZA32
C	625	ALA	-	expression tag	UNP Q7ZA32
C	626	LEU	-	expression tag	UNP Q7ZA32
C	627	GLU	-	expression tag	UNP Q7ZA32
C	628	HIS	-	expression tag	UNP Q7ZA32
C	629	HIS	-	expression tag	UNP Q7ZA32
C	630	HIS	-	expression tag	UNP Q7ZA32
C	631	HIS	-	expression tag	UNP Q7ZA32
C	632	HIS	-	expression tag	UNP Q7ZA32
C	633	HIS	-	expression tag	UNP Q7ZA32
D	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
D	167	ALA	HIS	engineered mutation	UNP Q7ZA32
D	623	ALA	-	expression tag	UNP Q7ZA32
D	624	ALA	-	expression tag	UNP Q7ZA32
D	625	ALA	-	expression tag	UNP Q7ZA32
D	626	LEU	-	expression tag	UNP Q7ZA32
D	627	GLU	-	expression tag	UNP Q7ZA32
D	628	HIS	-	expression tag	UNP Q7ZA32
D	629	HIS	-	expression tag	UNP Q7ZA32
D	630	HIS	-	expression tag	UNP Q7ZA32
D	631	HIS	-	expression tag	UNP Q7ZA32
D	632	HIS	-	expression tag	UNP Q7ZA32
D	633	HIS	-	expression tag	UNP Q7ZA32

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			12	6	1	5		
3	B	1	Total	C	F	O	0	0
			12	6	1	5		
3	C	1	Total	C	F	O	0	0
			12	6	1	5		
3	D	1	Total	C	F	O	0	0
			12	6	1	5		

- Molecule 4 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: $C_{24}H_{50}O_{13}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			16	10	6		
4	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	12	6	1	4	1	0	0
5	C	1	12	6	1	4	1	0	0

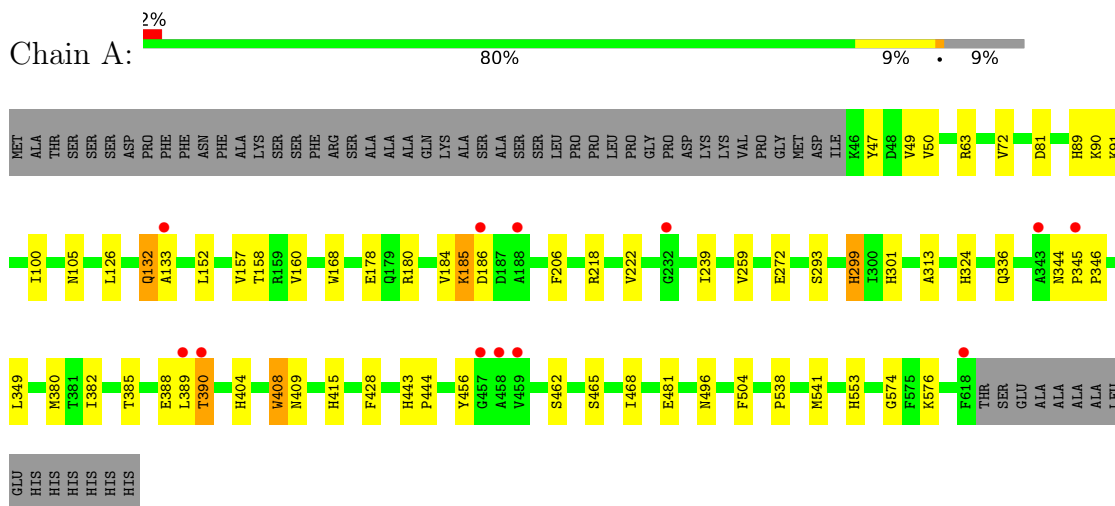
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	516	Total	O	0	0
			516	516		
6	B	518	Total	O	0	0
			518	518		
6	C	409	Total	O	0	0
			409	409		
6	D	323	Total	O	0	0
			323	323		

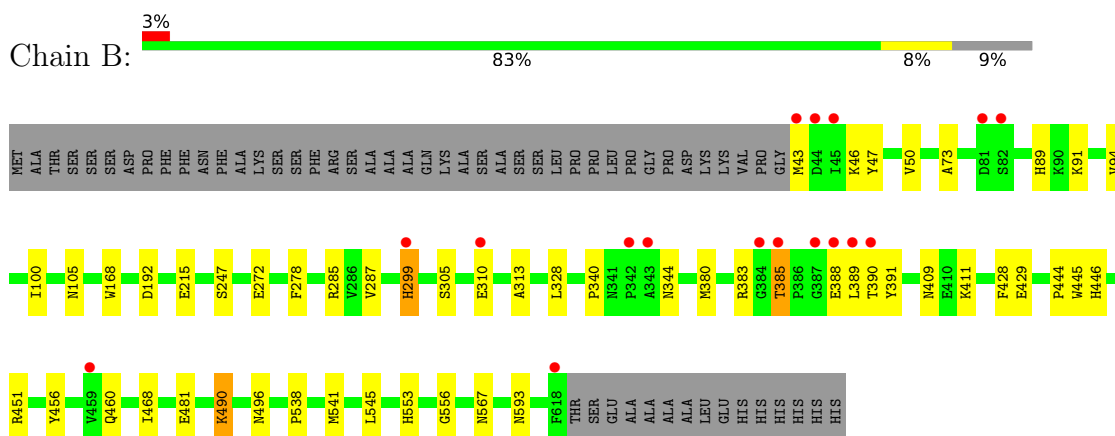
3 Residue-property plots [i](#)

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.

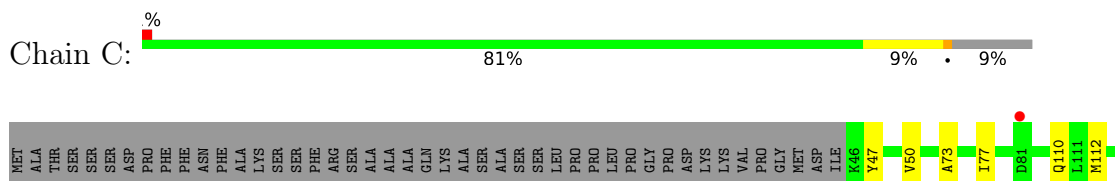
- Molecule 1: Pyranose 2-oxidase



- Molecule 1: Pyranose 2-oxidase



- Molecule 1: Pyranose 2-oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.29Å 102.48Å 137.42Å 90.00° 91.02° 90.00°	Depositor
Resolution (Å)	48.01 – 2.00 48.01 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.01-2.00) 98.2 (48.01-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.186 , 0.222 0.165 , 0.206	Depositor DCC
R_{free} test set	1846 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.018 for -k,-h,-l 0.014 for k,h,-l 0.023 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20233	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: MES, FAD, 2FG, 12P

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	1.37	12/4656 (0.3%)	1.13	10/6329 (0.2%)
1	B	1.32	11/4663 (0.2%)	1.12	6/6339 (0.1%)
1	C	1.23	9/4639 (0.2%)	1.11	10/6307 (0.2%)
1	D	1.11	3/4639 (0.1%)	1.05	2/6307 (0.0%)
All	All	1.26	35/18597 (0.2%)	1.10	28/25282 (0.1%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	HIS	CG-CD2	9.15	1.46	1.35
1	A	349	LEU	C-O	-8.93	1.19	1.23
1	A	553	HIS	CG-CD2	7.08	1.43	1.35
1	A	553	HIS	ND1-CE1	7.02	1.39	1.32
1	A	299	HIS	CG-CD2	6.99	1.43	1.35
1	A	443	HIS	CG-CD2	6.96	1.43	1.35
1	B	553	HIS	ND1-CE1	6.78	1.39	1.32
1	A	222	VAL	C-O	-6.42	1.16	1.24
1	A	415	HIS	CG-CD2	6.28	1.42	1.35
1	C	349	LEU	C-O	-6.27	1.21	1.23
1	C	425	PRO	C-O	-6.19	1.16	1.24
1	B	94	VAL	N-CA	-6.09	1.39	1.46
1	C	450	HIS	ND1-CE1	6.03	1.38	1.32
1	B	428	PHE	C-O	-5.98	1.17	1.24
1	B	299	HIS	ND1-CE1	5.89	1.38	1.32
1	C	443	HIS	CE1-NE2	5.89	1.38	1.32
1	C	132	GLN	CD-OE1	5.86	1.34	1.23
1	B	390	THR	CA-CB	5.76	1.60	1.53
1	C	299	HIS	CG-CD2	5.74	1.42	1.35
1	C	443	HIS	CG-CD2	5.72	1.42	1.35
1	A	301	HIS	ND1-CE1	5.60	1.38	1.32
1	B	385	THR	CA-C	5.59	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	443	HIS	CG-CD2	5.56	1.42	1.35
1	A	444	PRO	CA-C	5.45	1.58	1.53
1	B	446	HIS	CG-CD2	5.44	1.41	1.35
1	D	299	HIS	CG-CD2	5.41	1.41	1.35
1	B	89	HIS	CG-ND1	-5.30	1.32	1.38
1	A	89	HIS	CD2-NE2	-5.21	1.32	1.37
1	A	462	SER	N-CA	-5.20	1.39	1.46
1	B	305	SER	C-O	-5.18	1.17	1.24
1	A	132	GLN	CD-OE1	5.11	1.33	1.23
1	D	382	ILE	C-O	-5.08	1.18	1.24
1	B	446	HIS	CG-ND1	-5.07	1.32	1.38
1	C	478	GLU	CD-OE1	5.06	1.34	1.25
1	C	467	LEU	N-CA	-5.04	1.39	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	430	ASP	CA-C-N	-8.19	111.92	120.03
1	C	430	ASP	C-N-CA	-8.19	111.92	120.03
1	C	132	GLN	N-CA-C	7.22	120.43	109.23
1	C	345	PRO	CA-C-N	-7.14	113.32	120.31
1	C	345	PRO	C-N-CA	-7.14	113.32	120.31
1	B	168	TRP	N-CA-C	6.81	119.11	110.33
1	B	385	THR	CA-C-N	6.30	126.25	119.76
1	B	385	THR	C-N-CA	6.30	126.25	119.76
1	A	428	PHE	CA-C-N	-6.12	113.40	122.83
1	A	428	PHE	C-N-CA	-6.12	113.40	122.83
1	D	344	ASN	CB-CA-C	-6.01	104.40	110.65
1	A	168	TRP	N-CA-C	5.96	118.01	110.33
1	A	390	THR	N-CA-CB	-5.74	101.04	110.40
1	C	390	THR	CB-CA-C	-5.70	100.08	110.63
1	C	428	PHE	CA-C-N	-5.67	114.18	122.86
1	C	428	PHE	C-N-CA	-5.67	114.18	122.86
1	A	239	ILE	CA-C-N	-5.62	114.00	119.90
1	A	239	ILE	C-N-CA	-5.62	114.00	119.90
1	A	180	ARG	CA-C-N	-5.36	114.72	120.03
1	A	180	ARG	C-N-CA	-5.36	114.72	120.03
1	B	192	ASP	CB-CA-C	-5.19	102.17	110.79
1	B	46	LYS	N-CA-C	5.19	116.88	108.41
1	B	247	SER	N-CA-C	-5.19	103.45	108.07
1	C	77	ILE	CA-C-N	-5.16	117.84	122.43
1	C	77	ILE	C-N-CA	-5.16	117.84	122.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	47	TYR	N-CA-C	5.09	117.90	109.85
1	A	404	HIS	CA-C-N	5.03	125.00	120.03
1	A	404	HIS	C-N-CA	5.03	125.00	120.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4535	0	4392	36	0
1	B	4545	0	4399	27	0
1	C	4521	0	4375	42	0
1	D	4521	0	4375	35	0
2	A	53	0	29	0	0
2	B	53	0	29	0	0
2	C	53	0	29	0	0
2	D	53	0	29	1	0
3	A	12	0	11	0	0
3	B	12	0	11	0	0
3	C	12	0	11	0	0
3	D	12	0	11	0	0
4	A	16	0	21	0	0
4	B	32	0	42	0	0
4	D	13	0	16	0	0
5	A	12	0	13	3	0
5	C	12	0	13	0	0
6	A	516	0	0	6	0
6	B	518	0	0	4	0
6	C	409	0	0	6	0
6	D	323	0	0	5	0
All	All	20233	0	17806	137	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 4.

All (137) 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:C:481:GLU:HG2	6:C:1182:HOH:O	1.56	1.03
1:B:299:HIS:HB3	6:B:1206:HOH:O	1.65	0.97
1:C:126:LEU:CD1	1:C:132:GLN:HG3	1.95	0.96
1:D:612:ASN:HD22	1:D:612:ASN:N	1.61	0.91
1:C:126:LEU:HD12	1:C:132:GLN:HG3	1.48	0.90
1:D:611:GLN:C	1:D:612:ASN:HD22	1.80	0.88
1:C:126:LEU:CD1	1:C:132:GLN:CG	2.54	0.85
1:A:126:LEU:HD12	1:A:132:GLN:CG	2.15	0.77
1:B:299:HIS:NE2	1:B:310:GLU:HG3	2.01	0.76
1:C:126:LEU:HD13	1:C:132:GLN:CG	2.18	0.74
1:C:126:LEU:HD13	1:C:132:GLN:HG2	1.69	0.74
1:D:382:ILE:HD13	6:D:1146:HOH:O	1.87	0.73
1:A:126:LEU:HD12	1:A:132:GLN:HG3	1.69	0.73
1:D:385:THR:O	1:D:388:GLU:HG2	1.90	0.72
1:C:385:THR:OG1	1:C:388:GLU:HG2	1.94	0.67
1:A:382:ILE:HD12	6:A:1127:HOH:O	1.97	0.65
1:C:545:LEU:HD12	6:C:1157:HOH:O	1.97	0.65
1:D:49:VAL:HG22	1:D:315:VAL:HB	1.78	0.64
1:C:384:GLY:HA3	1:C:390:THR:HG22	1.80	0.63
1:A:132:GLN:HE22	5:A:804:MES:HN4	1.47	0.62
1:A:158:THR:HG22	1:A:160:VAL:HG22	1.82	0.62
1:A:388:GLU:HB2	1:A:390:THR:HG22	1.82	0.62
1:B:91:LYS:HD2	1:B:100:ILE:HD11	1.81	0.62
1:B:299:HIS:CD2	1:B:310:GLU:HG3	2.34	0.62
1:C:385:THR:OG1	1:C:388:GLU:CG	2.49	0.61
1:B:538:PRO:HG2	1:D:538:PRO:HG2	1.81	0.61
1:D:612:ASN:N	1:D:612:ASN:ND2	2.36	0.60
1:B:481:GLU:HG2	6:B:1190:HOH:O	1.99	0.60
1:C:299:HIS:NE2	1:C:310:GLU:HG2	2.17	0.60
1:A:299:HIS:HB3	6:A:1312:HOH:O	2.02	0.58
1:A:126:LEU:CD1	1:A:132:GLN:CG	2.81	0.58
1:A:481:GLU:HG2	6:A:1316:HOH:O	2.03	0.58
1:C:465:SER:HA	1:C:468:ILE:HD12	1.85	0.58
1:D:218:ARG:HG3	1:D:430:ASP:OD2	2.04	0.58
1:A:63:ARG:HD2	1:A:259:VAL:O	2.04	0.58
1:D:450:HIS:HD2	6:D:1034:HOH:O	1.87	0.57
6:C:1180:HOH:O	1:D:84:LEU:HD23	2.04	0.57
1:D:299:HIS:NE2	1:D:310:GLU:CG	2.68	0.57
1:B:299:HIS:NE2	1:B:310:GLU:CG	2.68	0.56
1:B:545:LEU:HD12	6:B:1341:HOH:O	2.05	0.56
1:D:299:HIS:HB3	6:D:1148:HOH:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:444:PRO:HD2	1:D:445:TRP:CZ3	2.41	0.56
1:B:380:MET:HE1	1:B:409:ASN:HB3	1.88	0.55
1:B:490:LYS:HD3	6:B:1232:HOH:O	2.06	0.55
1:D:450:HIS:CE1	1:D:472:ARG:HH11	2.24	0.55
1:A:388:GLU:CB	1:A:390:THR:HG22	2.36	0.55
1:C:450:HIS:HD2	6:C:852:HOH:O	1.89	0.55
1:A:91:LYS:HD2	1:A:100:ILE:HD11	1.89	0.55
1:D:299:HIS:NE2	1:D:310:GLU:HG2	2.22	0.54
1:B:383:ARG:O	1:B:391:TYR:HA	2.08	0.54
1:A:133:ALA:HB3	5:A:804:MES:H71	1.90	0.53
1:D:107:ILE:HG12	1:D:167:ALA:HB1	1.90	0.52
1:A:538:PRO:HG2	1:C:538:PRO:HG2	1.92	0.52
1:A:456:TYR:CD1	1:A:541:MET:HE2	2.45	0.52
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.92	0.51
1:C:158:THR:HG22	1:C:160:VAL:HG22	1.93	0.51
1:C:50:VAL:HG13	1:C:313:ALA:HB2	1.93	0.50
1:B:43:MET:HG3	1:B:278:PHE:CE1	2.47	0.49
1:D:611:GLN:C	1:D:612:ASN:ND2	2.59	0.49
1:B:215:GLU:O	1:B:411:LYS:NZ	2.46	0.49
5:A:804:MES:H22	1:D:149:LEU:HD22	1.95	0.48
1:B:451[A]:ARG:HD3	1:B:468:ILE:O	2.14	0.48
1:A:49:VAL:HB	1:A:72:VAL:HG22	1.95	0.48
1:C:299:HIS:NE2	1:C:310:GLU:CG	2.75	0.48
1:D:459:VAL:CG1	1:D:461:GLN:HE21	2.26	0.48
1:B:556:GLY:O	1:B:567:ASN:HA	2.13	0.48
1:C:382:ILE:HD13	6:C:1177:HOH:O	2.14	0.48
1:B:460:GLN:CD	1:B:460:GLN:C	2.81	0.47
1:C:218:ARG:HG3	1:C:430:ASP:OD2	2.14	0.47
1:C:390:THR:HG22	1:C:390:THR:O	2.13	0.47
1:B:328:LEU:HD23	1:B:328:LEU:C	2.40	0.47
1:C:537:LEU:HB3	1:C:538:PRO:HD2	1.96	0.47
1:A:47:TYR:O	1:A:313:ALA:HA	2.15	0.46
1:C:324:HIS:HD2	6:C:859:HOH:O	1.98	0.46
1:A:336:GLN:NE2	1:A:344:ASN:O	2.49	0.46
1:D:380:MET:HE1	1:D:409:ASN:HB3	1.96	0.46
1:B:389:LEU:HA	1:B:389:LEU:HD12	1.68	0.46
1:B:456:TYR:CD1	1:B:541:MET:HE2	2.51	0.46
1:B:47:TYR:CE2	1:B:73:ALA:HB2	2.51	0.45
1:D:218:ARG:HD2	6:D:916:HOH:O	2.16	0.45
1:B:285:ARG:NH2	1:B:287:VAL:HG22	2.32	0.45
1:C:349:LEU:HD22	1:C:565:CYS:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:TYR:CG	1:D:541:MET:HE2	2.52	0.45
1:C:110:GLN:C	1:C:112:MET:HE2	2.42	0.45
1:A:158:THR:CG2	1:A:160:VAL:HG22	2.47	0.44
1:D:159:ARG:HA	2:D:801:FAD:O2B	2.17	0.44
1:D:456:TYR:CD1	1:D:541:MET:HE2	2.52	0.44
1:C:380:MET:HE1	1:C:409:ASN:HB3	2.00	0.43
1:B:456:TYR:CG	1:B:541:MET:HE2	2.53	0.43
1:D:247:SER:HB2	1:D:248:PRO:CD	2.48	0.43
1:D:289:ASN:HB3	1:D:296:GLU:OE2	2.19	0.43
1:A:345:PRO:HA	1:A:346:PRO:HD3	1.94	0.43
1:C:242:ALA:HB1	1:C:254:SER:HB2	2.01	0.43
1:D:82:SER:N	6:D:1039:HOH:O	2.50	0.43
1:C:457:GLY:O	1:C:458:ALA:C	2.62	0.43
1:A:389:LEU:HG	6:A:1292:HOH:O	2.18	0.43
1:A:185:LYS:O	1:A:186:ASP:HB2	2.19	0.43
1:C:383:ARG:NH1	1:C:390:THR:HG23	2.34	0.43
1:D:293:SER:HA	1:D:574:GLY:O	2.18	0.43
1:A:218:ARG:HD2	6:A:1009:HOH:O	2.19	0.42
1:A:456:TYR:CG	1:A:541:MET:HE2	2.53	0.42
1:A:380:MET:HE1	1:A:409:ASN:HB3	2.01	0.42
1:C:384:GLY:HA3	1:C:390:THR:CG2	2.48	0.42
1:A:157:VAL:HG21	1:A:324:HIS:HE1	1.84	0.42
1:B:385:THR:O	1:B:388:GLU:HB2	2.18	0.42
1:C:182:LEU:HA	1:C:182:LEU:HD23	1.74	0.42
1:D:91:LYS:HD2	1:D:100:ILE:HD11	2.01	0.42
1:D:459:VAL:HG13	1:D:461:GLN:HE21	1.84	0.42
1:A:152:LEU:HD21	1:A:504:PHE:CD1	2.55	0.42
1:B:50:VAL:HG13	1:B:313:ALA:HB2	2.00	0.42
1:C:385:THR:OG1	1:C:388:GLU:HG3	2.19	0.42
1:D:363:PHE:HA	1:D:471:TRP:O	2.20	0.42
1:A:408:TRP:C	1:A:408:TRP:CD1	2.98	0.42
1:D:354:SER:OG	1:D:484:LYS:NZ	2.51	0.42
1:D:556:GLY:O	1:D:567:ASN:HA	2.20	0.41
1:C:143:ASN:HA	1:C:144:PRO:HD2	1.95	0.41
1:D:349:LEU:HD11	1:D:572:VAL:HG13	2.03	0.41
1:A:81:ASP:OD2	1:A:90:LYS:NZ	2.49	0.41
1:A:126:LEU:CD1	1:A:132:GLN:CD	2.93	0.41
1:C:384:GLY:CA	1:C:390:THR:CG2	2.99	0.41
1:B:328:LEU:HD23	1:B:328:LEU:O	2.21	0.41
1:C:328:LEU:C	1:C:328:LEU:HD23	2.46	0.41
1:C:341:ASN:HA	1:C:342:PRO:HD2	1.95	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:GLY:HA2	1:C:390:THR:HG21	2.03	0.41
1:A:465[B]:SER:HA	1:A:468:ILE:HD12	2.03	0.41
1:B:444:PRO:HD2	1:B:445:TRP:CZ3	2.55	0.41
1:A:105:ASN:HB3	1:B:105:ASN:O	2.21	0.41
1:A:388:GLU:HB2	1:A:390:THR:CG2	2.49	0.41
1:A:576:LYS:HG3	6:A:1362:HOH:O	2.21	0.41
1:C:317:VAL:HG12	1:C:319:THR:HG23	2.03	0.41
1:C:408:TRP:CD1	1:C:408:TRP:C	2.98	0.41
1:A:293:SER:HA	1:A:574:GLY:O	2.21	0.41
1:C:173:PRO:HG2	1:C:592:ALA:HB1	2.02	0.41
1:C:384:GLY:CA	1:C:390:THR:HG22	2.49	0.41
1:C:47:TYR:CD2	1:C:73:ALA:HB2	2.56	0.40
1:D:284:GLU:C	1:D:328:LEU:CD1	2.94	0.40
1:C:471:TRP:CH2	1:C:526:SER:HA	2.56	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	574/633 (91%)	557 (97%)	17 (3%)	0	100	100
1	B	575/633 (91%)	559 (97%)	16 (3%)	0	100	100
1	C	572/633 (90%)	553 (97%)	19 (3%)	0	100	100
1	D	572/633 (90%)	554 (97%)	18 (3%)	0	100	100
All	All	2293/2532 (91%)	2223 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	503/547 (92%)	495 (98%)	8 (2%)	55	62
1	B	504/547 (92%)	497 (99%)	7 (1%)	59	66
1	C	501/547 (92%)	494 (99%)	7 (1%)	59	66
1	D	501/547 (92%)	495 (99%)	6 (1%)	63	70
All	All	2009/2188 (92%)	1981 (99%)	28 (1%)	59	66

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
1	A	184	VAL
1	A	185	LYS
1	A	206	PHE
1	A	272	GLU
1	A	385	THR
1	A	408	TRP
1	A	496	ASN
1	B	272	GLU
1	B	340	PRO
1	B	344	ASN
1	B	429	GLU
1	B	490	LYS
1	B	496	ASN
1	B	593	ASN
1	C	206	PHE
1	C	228	GLU
1	C	408	TRP
1	C	459	VAL
1	C	462	SER
1	C	534	PRO
1	C	593	ASN
1	D	204	SER
1	D	272	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	328	LEU
1	D	408	TRP
1	D	496	ASN
1	D	612	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	224	ASN
1	A	257	ASN
1	A	276	ASN
1	A	418	GLN
1	A	419	HIS
1	A	612	ASN
1	B	105	ASN
1	B	257	ASN
1	B	276	ASN
1	B	365	GLN
1	B	418	GLN
1	B	419	HIS
1	C	105	ASN
1	C	132	GLN
1	C	257	ASN
1	C	324	HIS
1	C	327	GLN
1	C	419	HIS
1	C	450	HIS
1	C	461	GLN
1	D	324	HIS
1	D	365	GLN
1	D	450	HIS
1	D	461	GLN
1	D	612	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	D	801	-	58,58,58	1.52	11 (18%)	85,89,89	2.26	34 (40%)
4	12P	B	803	-	15,15,36	0.62	0	14,14,35	0.39	0
5	MES	A	804	-	12,12,12	2.09	1 (8%)	15,16,16	2.61	3 (20%)
3	2FG	D	802	-	12,12,12	1.33	2 (16%)	16,17,17	2.01	3 (18%)
3	2FG	B	802	-	12,12,12	0.98	1 (8%)	16,17,17	1.40	3 (18%)
3	2FG	C	703	-	12,12,12	1.19	1 (8%)	16,17,17	1.55	1 (6%)
2	FAD	A	801	-	58,58,58	1.63	9 (15%)	85,89,89	2.34	28 (32%)
2	FAD	B	801	-	58,58,58	1.65	13 (22%)	85,89,89	2.22	28 (32%)
3	2FG	A	802	-	12,12,12	1.06	2 (16%)	16,17,17	1.88	6 (37%)
4	12P	A	803	-	15,15,36	0.67	0	14,14,35	0.52	0
5	MES	C	701	-	12,12,12	1.87	1 (8%)	15,16,16	1.94	4 (26%)
2	FAD	C	702	-	58,58,58	1.29	7 (12%)	85,89,89	2.38	27 (31%)
4	12P	B	804	-	15,15,36	0.53	0	14,14,35	0.57	0
4	12P	D	803	-	12,12,36	0.67	0	11,11,35	0.46	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
2	FAD	D	801	-	-	3/34/50/50	0/6/6/6
4	12P	B	803	-	-	4/13/13/34	-
5	MES	A	804	-	-	0/6/14/14	0/1/1/1
3	2FG	D	802	-	-	1/2/22/22	0/1/1/1
3	2FG	B	802	-	-	1/2/22/22	0/1/1/1
3	2FG	C	703	-	-	1/2/22/22	0/1/1/1
2	FAD	A	801	-	-	1/34/50/50	0/6/6/6
2	FAD	B	801	-	-	3/34/50/50	0/6/6/6
3	2FG	A	802	-	-	1/2/22/22	0/1/1/1
4	12P	A	803	-	-	3/13/13/34	-
5	MES	C	701	-	-	0/6/14/14	0/1/1/1
2	FAD	C	702	-	-	2/34/50/50	0/6/6/6
4	12P	B	804	-	-	4/13/13/34	-
4	12P	D	803	-	-	2/10/10/34	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	PA-O3P	6.68	1.66	1.59
5	A	804	MES	C8-S	-6.04	1.69	1.77
5	C	701	MES	C8-S	-5.04	1.70	1.77
2	B	801	FAD	PA-O3P	4.89	1.64	1.59
2	B	801	FAD	C6-C5X	3.87	1.45	1.40
2	D	801	FAD	O4B-C4B	-3.87	1.36	1.45
2	D	801	FAD	P-O3P	3.81	1.63	1.59
2	B	801	FAD	C2B-C3B	-3.67	1.43	1.53
2	D	801	FAD	C8A-N9A	-3.38	1.31	1.37
2	B	801	FAD	O3B-C3B	-3.32	1.34	1.43
2	A	801	FAD	P-O3P	3.24	1.63	1.59
2	B	801	FAD	C8A-N9A	-3.06	1.32	1.37
2	A	801	FAD	C2B-C3B	-3.04	1.45	1.53
2	A	801	FAD	C6-C5X	3.04	1.44	1.40
2	A	801	FAD	O4B-C4B	-2.99	1.38	1.45
2	C	702	FAD	P-O3P	2.94	1.62	1.59
2	B	801	FAD	C5A-N7A	-2.86	1.33	1.39
2	A	801	FAD	O3B-C3B	-2.73	1.36	1.43
3	C	703	2FG	F2-C2	-2.66	1.35	1.40
3	D	802	2FG	C4-C5	2.64	1.58	1.53
2	A	801	FAD	C2A-N1A	2.49	1.38	1.33
2	B	801	FAD	C7M-C7	2.45	1.55	1.51
2	C	702	FAD	C8M-C8	2.41	1.55	1.51
2	B	801	FAD	C4A-N9A	-2.40	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FAD	C5X-N5	-2.39	1.35	1.39
2	C	702	FAD	C3B-C4B	-2.39	1.46	1.53
3	A	802	2FG	F2-C2	-2.33	1.35	1.40
2	B	801	FAD	C2A-N3A	2.31	1.38	1.33
3	B	802	2FG	F2-C2	-2.31	1.35	1.40
3	D	802	2FG	C2-C3	2.27	1.54	1.52
2	D	801	FAD	C2-N3	-2.25	1.34	1.39
2	D	801	FAD	C4-N3	-2.24	1.34	1.38
2	D	801	FAD	O2B-C2B	-2.23	1.37	1.43
2	C	702	FAD	O4B-C4B	-2.23	1.40	1.45
2	C	702	FAD	C5X-N5	-2.20	1.35	1.39
2	D	801	FAD	C5X-N5	-2.20	1.35	1.39
2	B	801	FAD	C8A-N7A	2.19	1.35	1.31
2	D	801	FAD	C10-N1	2.19	1.37	1.33
2	A	801	FAD	O2B-C2B	-2.18	1.37	1.43
2	B	801	FAD	C9-C8	2.17	1.42	1.39
2	D	801	FAD	C2B-C3B	-2.17	1.47	1.53
2	D	801	FAD	PA-O3P	2.14	1.61	1.59
3	A	802	2FG	C2-C1	-2.12	1.50	1.52
2	C	702	FAD	C6-C5X	2.10	1.43	1.40
2	C	702	FAD	C4-N3	-2.06	1.35	1.38
2	B	801	FAD	C10-N1	2.06	1.37	1.33
2	D	801	FAD	C1'-C2'	-2.05	1.49	1.52
2	A	801	FAD	C10-N1	2.05	1.37	1.33

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	MES	O2S-S-C8	7.98	118.79	106.73
2	A	801	FAD	C4A-N9A-C8A	7.30	113.41	105.74
2	B	801	FAD	C4A-N9A-C8A	7.00	113.08	105.74
2	A	801	FAD	N9A-C8A-N7A	-6.66	104.48	113.94
3	D	802	2FG	F2-C2-C3	6.28	114.25	108.81
2	D	801	FAD	C4A-N9A-C8A	6.06	112.11	105.74
2	B	801	FAD	N9A-C8A-N7A	-5.74	105.80	113.94
2	D	801	FAD	O4B-C1B-N9A	5.72	119.08	108.09
2	C	702	FAD	N9A-C8A-N7A	-5.59	106.01	113.94
2	A	801	FAD	N3A-C2A-N1A	-5.57	120.14	128.58
2	C	702	FAD	C4-N3-C2	5.50	135.42	125.64
2	C	702	FAD	C2B-C1B-N9A	5.43	126.80	113.30
2	B	801	FAD	N3A-C2A-N1A	-5.32	120.53	128.58
2	C	702	FAD	N3A-C2A-N1A	-5.31	120.54	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	C4-C4X-N5	5.26	125.47	118.21
3	C	703	2FG	F2-C2-C3	-5.13	104.37	108.81
5	C	701	MES	O3S-S-C8	5.10	115.98	106.00
2	C	702	FAD	C5A-C4A-N3A	-5.04	119.78	126.72
2	C	702	FAD	O4B-C1B-N9A	5.02	117.73	108.09
2	B	801	FAD	N3-C2-N1	-4.97	108.93	119.50
2	C	702	FAD	C4A-N9A-C8A	4.91	110.89	105.74
2	C	702	FAD	C5A-N7A-C8A	4.84	111.06	103.45
2	C	702	FAD	O3B-C3B-C4B	4.71	124.62	111.08
2	A	801	FAD	O4B-C1B-N9A	4.53	116.80	108.09
2	D	801	FAD	N9A-C8A-N7A	-4.50	107.56	113.94
2	D	801	FAD	C1B-N9A-C8A	-4.40	117.34	127.09
3	A	802	2FG	F2-C2-C1	4.39	112.73	107.81
2	B	801	FAD	O4B-C4B-C5B	4.28	123.05	109.33
2	A	801	FAD	C1B-N9A-C8A	-4.25	117.66	127.09
2	A	801	FAD	C10-N1-C2	4.23	126.02	116.85
2	A	801	FAD	C4-N3-C2	4.23	133.16	125.64
2	D	801	FAD	N3A-C2A-N1A	-4.22	122.20	128.58
2	B	801	FAD	C2B-C1B-N9A	4.20	123.73	113.30
2	C	702	FAD	C1B-N9A-C8A	-4.17	117.85	127.09
2	C	702	FAD	N3A-C4A-N9A	4.13	134.18	127.17
5	A	804	MES	O2S-S-O1S	-4.09	100.53	113.82
2	A	801	FAD	C2B-C1B-N9A	4.08	123.44	113.30
2	A	801	FAD	C5A-N7A-C8A	4.07	109.85	103.45
5	A	804	MES	O1S-S-C8	4.00	112.77	106.73
2	D	801	FAD	O2B-C2B-C1B	3.97	123.78	110.10
2	B	801	FAD	O4-C4-C4X	-3.97	116.05	126.53
2	D	801	FAD	C2B-C1B-N9A	3.93	123.06	113.30
2	D	801	FAD	C6A-C5A-C4A	3.91	122.52	117.18
2	C	702	FAD	O2B-C2B-C3B	3.87	124.22	111.82
2	C	702	FAD	C4A-C5A-N7A	-3.79	106.25	110.58
2	A	801	FAD	N3A-C4A-N9A	3.76	133.57	127.17
2	A	801	FAD	N3-C2-N1	-3.60	111.84	119.50
2	C	702	FAD	C2A-N3A-C4A	3.57	120.55	111.83
2	B	801	FAD	C9A-C5X-N5	-3.54	118.70	122.45
2	C	702	FAD	O2A-PA-O3P	3.54	116.84	107.27
2	D	801	FAD	O2A-PA-O1A	3.42	128.37	112.44
2	B	801	FAD	O2-C2-N3	3.41	125.12	118.58
2	A	801	FAD	C9A-C5X-N5	-3.41	118.84	122.45
2	D	801	FAD	O3P-PA-O1A	-3.38	100.54	110.70
2	C	702	FAD	C4X-C4-N3	-3.35	104.74	113.25
2	A	801	FAD	O4-C4-N3	3.32	126.35	120.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	C5B-C4B-C3B	3.30	127.09	115.21
2	A	801	FAD	O4B-C4B-C5B	3.26	119.79	109.33
2	A	801	FAD	O4B-C4B-C3B	3.24	111.59	105.15
2	D	801	FAD	O3B-C3B-C4B	3.23	120.37	111.08
2	D	801	FAD	N3A-C4A-N9A	3.22	132.65	127.17
2	A	801	FAD	O2P-P-O3P	-3.22	98.58	107.27
2	B	801	FAD	C1B-N9A-C8A	-3.19	120.01	127.09
2	D	801	FAD	C2A-N1A-C6A	3.19	123.97	118.73
2	C	702	FAD	N3-C2-N1	-3.16	112.79	119.50
2	D	801	FAD	C5A-N7A-C8A	3.13	108.37	103.45
2	B	801	FAD	C4X-C10-N1	-3.12	116.93	124.59
2	C	702	FAD	C4-C4X-C10	3.06	122.19	116.93
2	D	801	FAD	O2P-P-O3P	-3.02	99.10	107.27
2	B	801	FAD	O2B-C2B-C1B	3.00	120.44	110.10
2	C	702	FAD	C5B-C4B-C3B	2.98	125.95	115.21
2	B	801	FAD	C5A-N7A-C8A	2.98	108.13	103.45
2	D	801	FAD	O4B-C4B-C3B	2.97	111.04	105.15
2	B	801	FAD	N3A-C4A-N9A	2.87	132.05	127.17
2	A	801	FAD	O2B-C2B-C3B	2.87	121.00	111.82
2	B	801	FAD	O2P-P-O1P	2.84	125.67	112.44
2	A	801	FAD	C2A-N3A-C4A	2.81	118.70	111.83
2	D	801	FAD	C5A-C4A-N3A	-2.81	122.84	126.72
2	D	801	FAD	O4B-C4B-C5B	2.79	118.26	109.33
2	D	801	FAD	C4A-C5A-N7A	-2.78	107.40	110.58
2	D	801	FAD	O4-C4-C4X	-2.78	119.19	126.53
2	B	801	FAD	C10-N1-C2	2.77	122.86	116.85
2	B	801	FAD	C4'-C3'-C2'	-2.77	108.95	113.57
2	B	801	FAD	C2A-N1A-C6A	2.74	123.23	118.73
3	A	802	2FG	C1-C2-C3	-2.72	106.65	110.69
5	C	701	MES	O3S-S-O1S	-2.66	104.74	111.40
2	A	801	FAD	C5A-C4A-N3A	-2.64	123.09	126.72
2	B	801	FAD	O3B-C3B-C4B	2.62	118.62	111.08
2	A	801	FAD	C4X-C10-N1	-2.56	118.31	124.59
2	A	801	FAD	C5X-C9A-N10	2.56	120.28	117.97
2	A	801	FAD	O2B-C2B-C1B	2.55	118.90	110.10
2	C	702	FAD	O2B-C2B-C1B	2.55	118.87	110.10
5	C	701	MES	O1S-S-C8	2.54	110.56	106.73
3	B	802	2FG	O5-C5-C6	2.54	112.73	106.44
3	D	802	2FG	O3-C3-C2	-2.53	104.94	109.63
2	B	801	FAD	O2P-P-O3P	-2.53	100.44	107.27
2	B	801	FAD	O4B-C1B-N9A	2.50	112.90	108.09
2	C	702	FAD	C4-C4X-N5	-2.47	114.79	118.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	O4'-C4'-C3'	2.43	114.93	109.25
2	C	702	FAD	C8M-C8-C9	2.40	123.79	119.57
2	A	801	FAD	C5A-C4A-N9A	-2.37	103.23	105.81
2	D	801	FAD	O2A-PA-O3P	2.36	113.65	107.27
2	A	801	FAD	C5B-C4B-C3B	2.35	123.69	115.21
2	C	702	FAD	C6A-C5A-C4A	2.34	120.38	117.18
2	C	702	FAD	O4B-C4B-C5B	2.34	116.82	109.33
3	A	802	2FG	O4-C4-C3	-2.32	104.91	110.38
2	B	801	FAD	O2'-C2'-C3'	2.31	114.66	109.25
2	D	801	FAD	C4'-C3'-C2'	-2.30	109.74	113.57
2	D	801	FAD	O4B-C1B-C2B	2.30	111.54	106.62
3	D	802	2FG	O6-C6-C5	-2.27	103.62	111.33
2	A	801	FAD	C8M-C8-C7	-2.26	116.14	120.76
2	B	801	FAD	C6A-C5A-C4A	2.26	120.26	117.18
3	A	802	2FG	O1-C1-O5	2.25	117.09	110.41
3	A	802	2FG	F2-C2-C3	2.25	110.76	108.81
3	A	802	2FG	O3-C3-C4	2.24	115.67	110.38
2	A	801	FAD	C5'-C4'-C3'	-2.23	108.01	112.22
2	A	801	FAD	C2A-N1A-C6A	2.22	122.37	118.73
2	D	801	FAD	C4-C4X-C10	-2.22	113.13	116.93
2	D	801	FAD	C4B-O4B-C1B	-2.21	104.59	109.47
2	C	702	FAD	C4X-C10-N10	2.21	119.64	116.48
2	D	801	FAD	N3-C2-N1	-2.19	114.85	119.50
3	B	802	2FG	O1-C1-O5	2.18	116.88	110.41
2	B	801	FAD	C2A-N3A-C4A	2.18	117.14	111.83
2	B	801	FAD	C10-C4X-N5	-2.16	120.39	124.81
2	C	702	FAD	C8M-C8-C7	-2.16	116.35	120.76
2	D	801	FAD	O2B-C2B-C3B	2.14	118.69	111.82
2	D	801	FAD	C10-N1-C2	2.13	121.46	116.85
2	B	801	FAD	C5A-C4A-N3A	-2.12	123.80	126.72
2	A	801	FAD	C3B-C2B-C1B	2.12	105.47	101.46
2	D	801	FAD	O4'-C4'-C5'	2.11	114.65	109.99
2	C	702	FAD	O2-C2-N3	2.11	122.63	118.58
2	B	801	FAD	O4-C4-N3	2.08	124.03	120.11
5	C	701	MES	O2S-S-O1S	-2.06	107.13	113.82
2	D	801	FAD	C7M-C7-C6	-2.04	115.98	119.57
3	B	802	2FG	C1-C2-C3	-2.04	107.66	110.69
2	D	801	FAD	C9-C8-C7	-2.03	116.71	119.69
2	D	801	FAD	O2P-P-O1P	2.01	121.80	112.44

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	PA-O3P-P-O5'
4	A	803	12P	O13-C14-C15-O16
4	B	803	12P	O13-C14-C15-O16
3	B	802	2FG	O5-C5-C6-O6
3	C	703	2FG	O5-C5-C6-O6
3	A	802	2FG	O5-C5-C6-O6
2	D	801	FAD	O4B-C4B-C5B-O5B
4	A	803	12P	O7-C8-C9-O10
4	B	804	12P	O10-C11-C12-O13
3	D	802	2FG	O5-C5-C6-O6
2	B	801	FAD	P-O3P-PA-O1A
4	D	803	12P	O10-C11-C12-O13
4	B	804	12P	O1-C2-C3-O4
2	C	702	FAD	PA-O3P-P-O5'
4	A	803	12P	O1-C2-C3-O4
4	B	804	12P	O13-C14-C15-O16
4	D	803	12P	C8-C9-O10-C11
4	B	803	12P	C8-C9-O10-C11
2	B	801	FAD	P-O3P-PA-O2A
4	B	804	12P	C5-C6-O7-C8
4	B	803	12P	C15-C14-O13-C12
4	B	803	12P	C11-C12-O13-C14
2	C	702	FAD	P-O3P-PA-O2A
2	D	801	FAD	P-O3P-PA-O2A
2	A	801	FAD	O4B-C4B-C5B-O5B

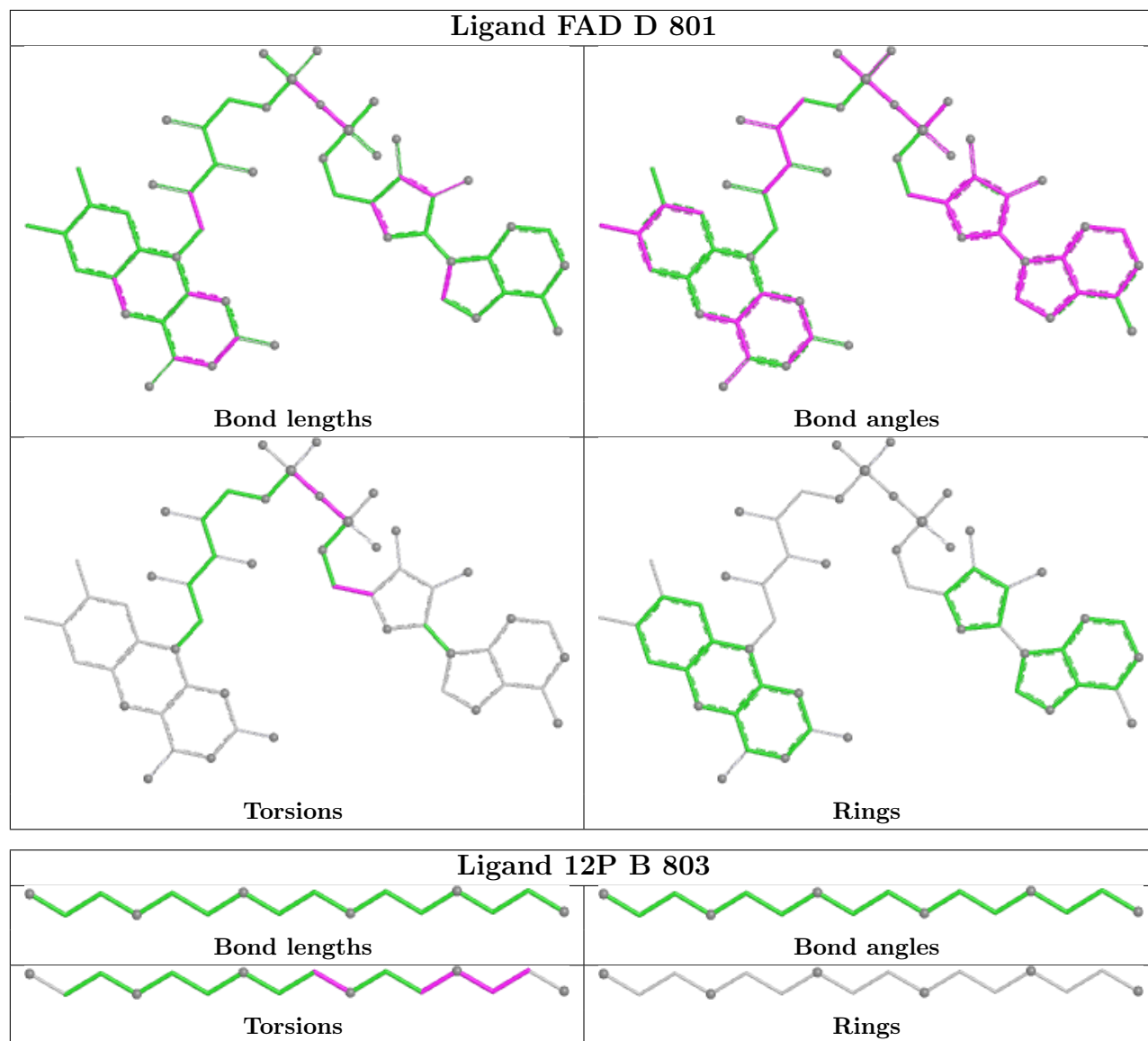
There are no ring outliers.

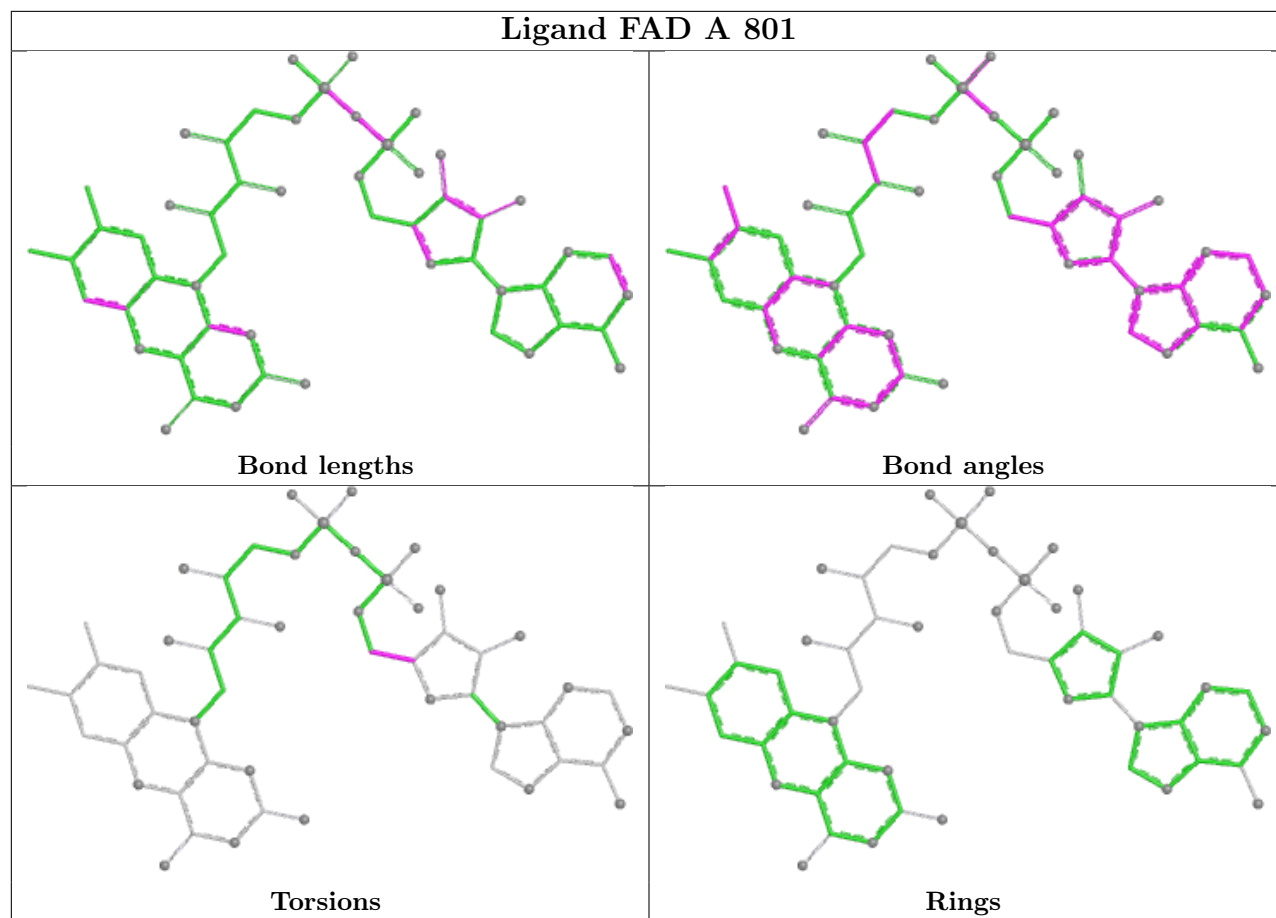
2 monomers are involved in 4 short contacts:

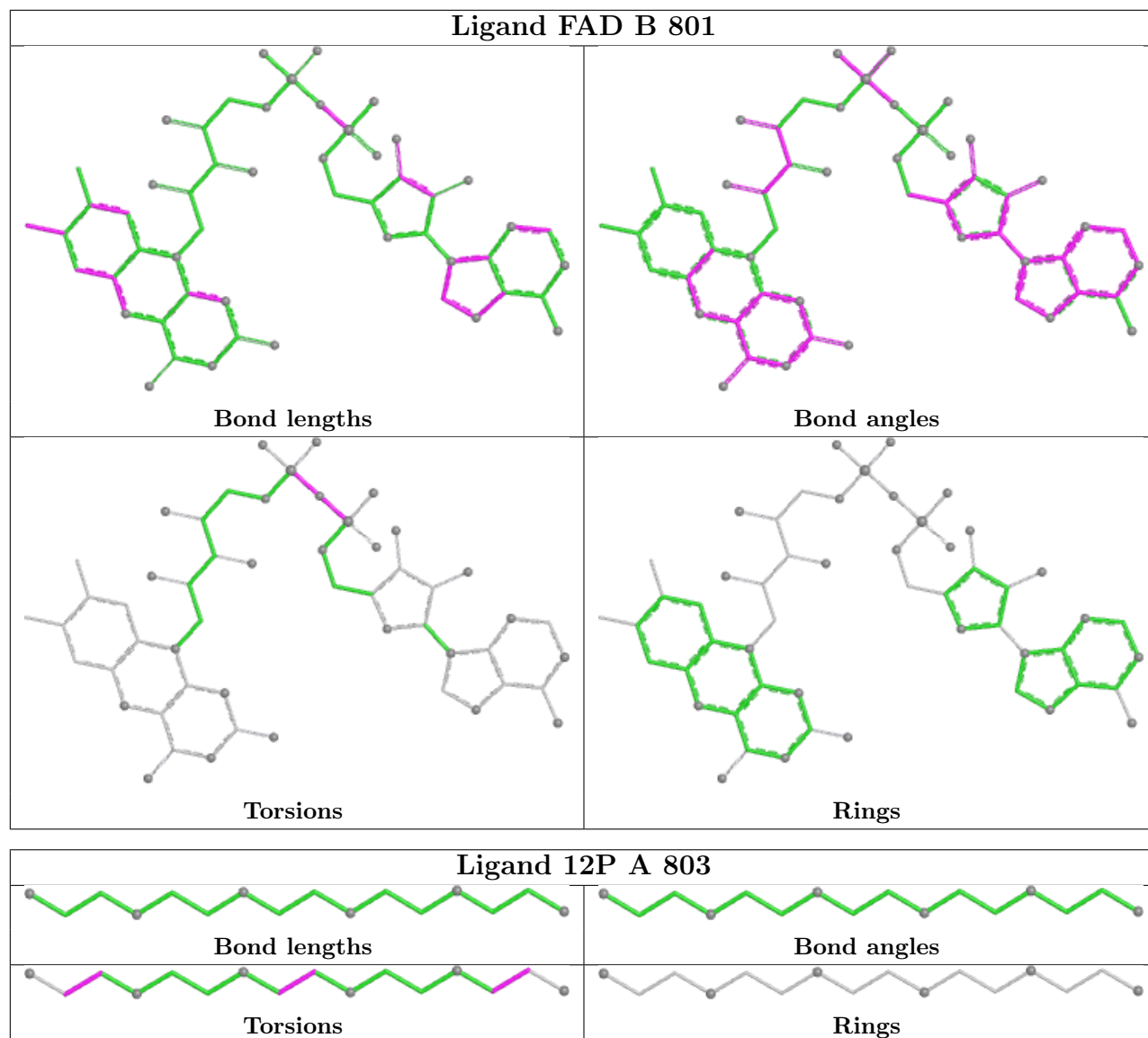
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	FAD	1	0
5	A	804	MES	3	0

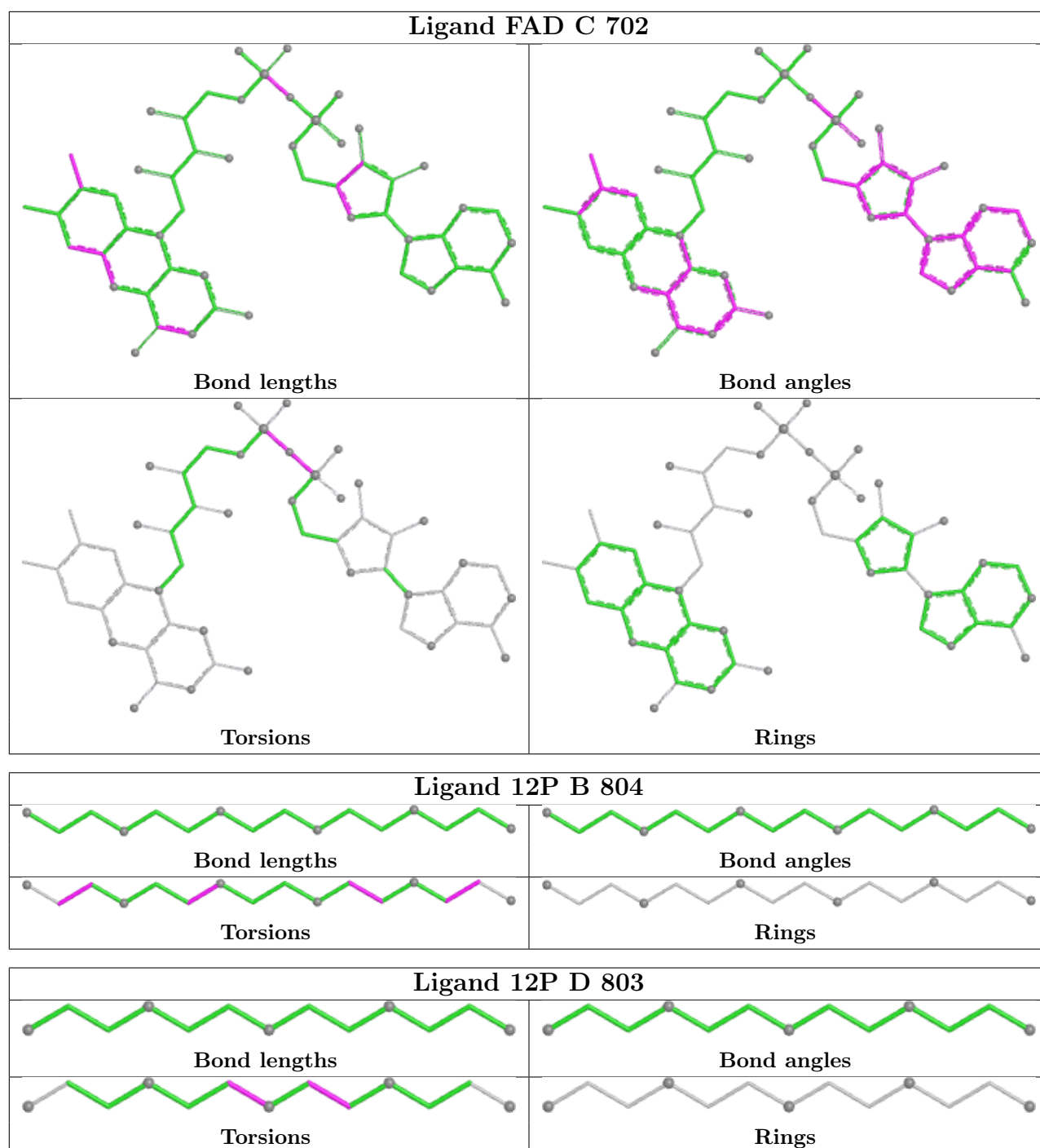
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

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	573/633 (90%)	-0.31	12 (2%) 63 63	12, 27, 45, 70	3 (0%)
1	B	576/633 (90%)	-0.24	17 (2%) 52 51	17, 27, 51, 76	1 (0%)
1	C	573/633 (90%)	-0.09	7 (1%) 76 76	19, 33, 55, 84	1 (0%)
1	D	573/633 (90%)	0.19	8 (1%) 73 73	19, 39, 61, 84	1 (0%)
All	All	2295/2532 (90%)	-0.11	44 (1%) 66 66	12, 31, 56, 84	6 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	459	VAL	4.5
1	D	82	SER	4.1
1	B	44	ASP	4.1
1	C	389	LEU	3.9
1	B	82	SER	3.8
1	B	389	LEU	3.7
1	D	618	PHE	3.6
1	B	459	VAL	3.5
1	D	459	VAL	3.5
1	B	390	THR	3.3
1	B	384	GLY	3.2
1	B	81	ASP	3.2
1	D	81	ASP	3.1
1	A	458	ALA	3.0
1	C	390	THR	3.0
1	B	299	HIS	3.0
1	A	389	LEU	2.9
1	A	232	GLY	2.9
1	B	45	ILE	2.9
1	C	385	THR	2.9
1	C	81	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	618	PHE	2.8
1	A	343	ALA	2.8
1	B	618	PHE	2.7
1	B	310	GLU	2.7
1	B	387	GLY	2.7
1	A	345	PRO	2.6
1	C	383	ARG	2.6
1	A	186	ASP	2.5
1	D	299	HIS	2.5
1	D	385	THR	2.5
1	D	291	LEU	2.5
1	B	43	MET	2.5
1	B	343	ALA	2.4
1	B	385	THR	2.4
1	A	133	ALA	2.3
1	A	618	PHE	2.2
1	B	342	PRO	2.2
1	A	188	ALA	2.2
1	B	388	GLU	2.1
1	C	459	VAL	2.1
1	A	457	GLY	2.1
1	D	457	GLY	2.1
1	A	390	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Continued on next page...

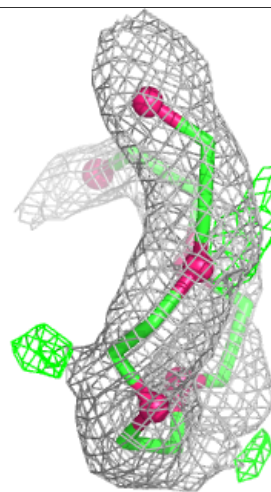
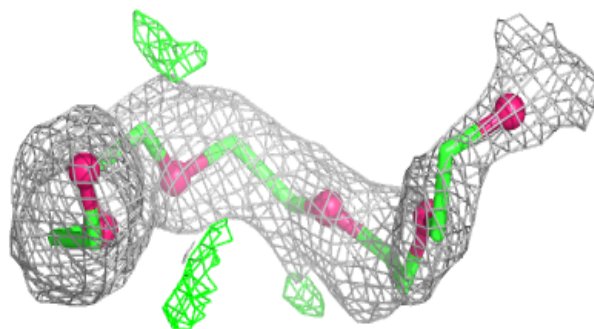
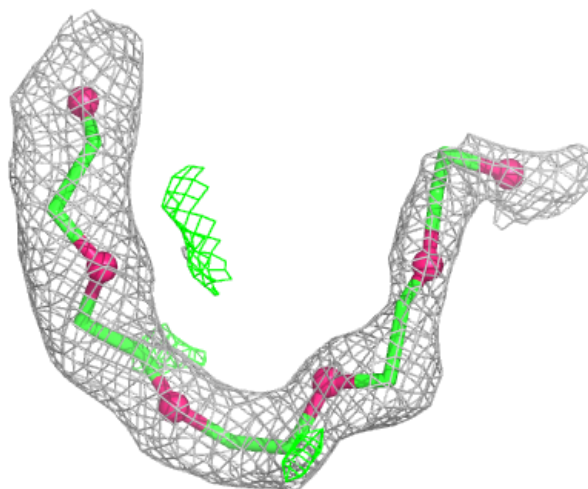
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	12P	B	803	16/37	0.86	0.17	45,53,70,70	0
4	12P	B	804	16/37	0.86	0.17	47,56,81,96	0
4	12P	D	803	13/37	0.87	0.15	52,60,63,64	0
5	MES	A	804	12/12	0.89	0.16	42,62,67,67	0
4	12P	A	803	16/37	0.90	0.13	45,56,63,65	0
5	MES	C	701	12/12	0.92	0.12	45,50,53,54	0
3	2FG	D	802	12/12	0.95	0.08	38,40,42,45	0
3	2FG	B	802	12/12	0.96	0.07	32,34,41,42	0
3	2FG	A	802	12/12	0.96	0.07	29,33,35,44	0
3	2FG	C	703	12/12	0.97	0.07	36,39,44,49	0
2	FAD	D	801	53/53	0.97	0.07	27,32,36,38	0
2	FAD	C	702	53/53	0.98	0.05	22,26,32,34	0
2	FAD	A	801	53/53	0.99	0.05	18,20,24,26	0
2	FAD	B	801	53/53	0.99	0.04	18,22,26,27	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.

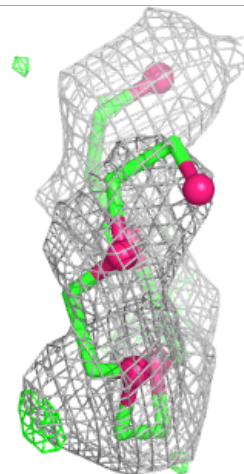
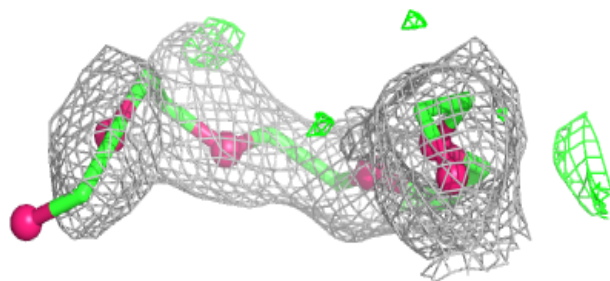
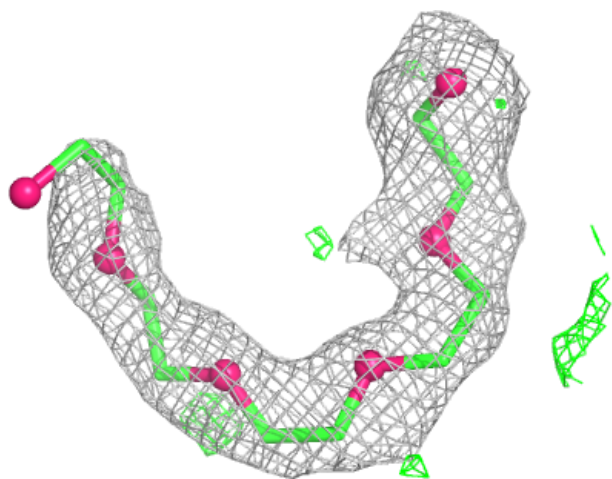
Electron density around 12P B 803:

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



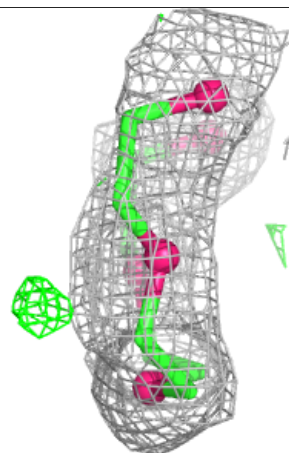
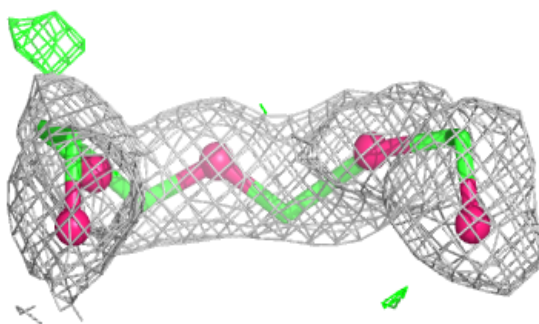
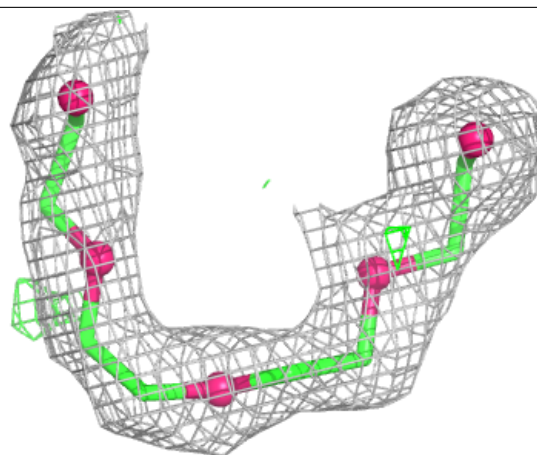
Electron density around 12P B 804:

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



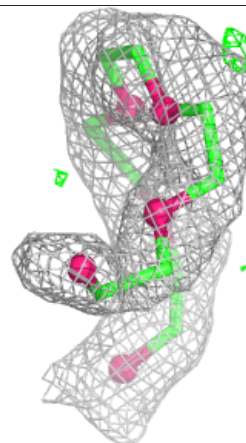
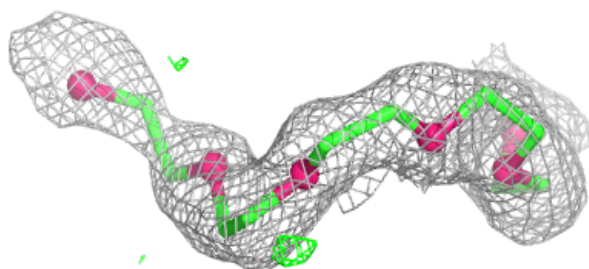
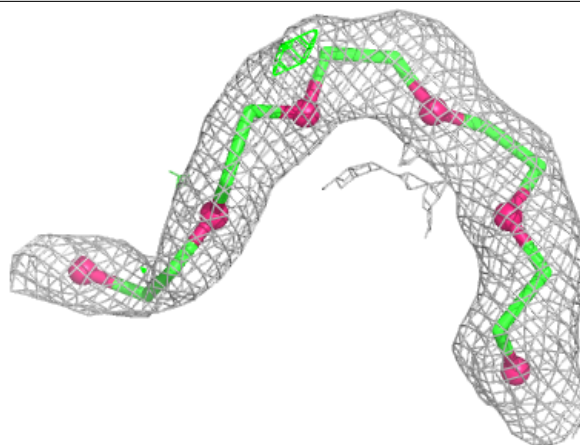
Electron density around 12P D 803:

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

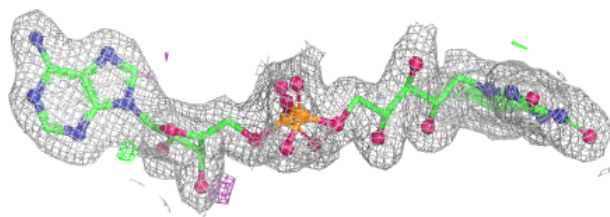
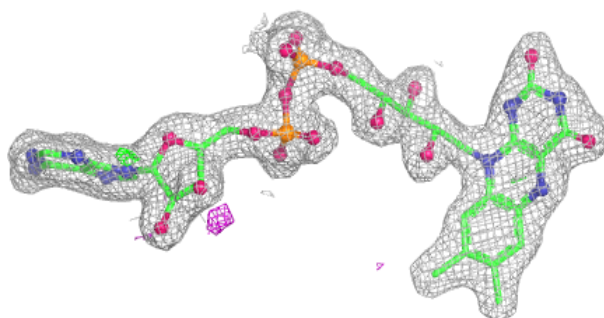


Electron density around 12P A 803:

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

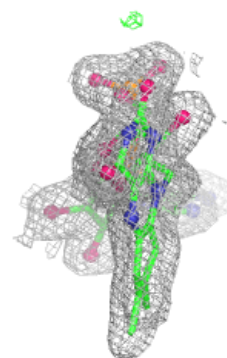
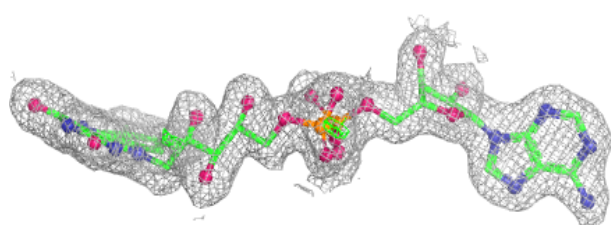
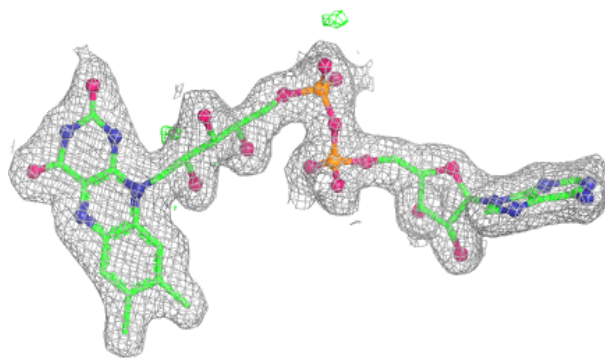
**Electron density around FAD D 801:**

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

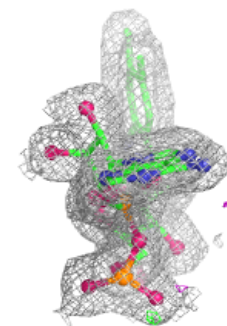
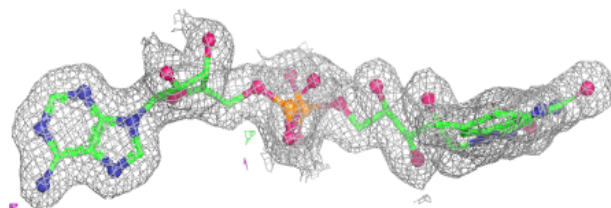
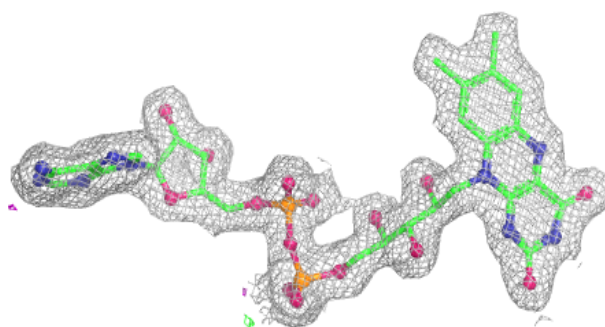


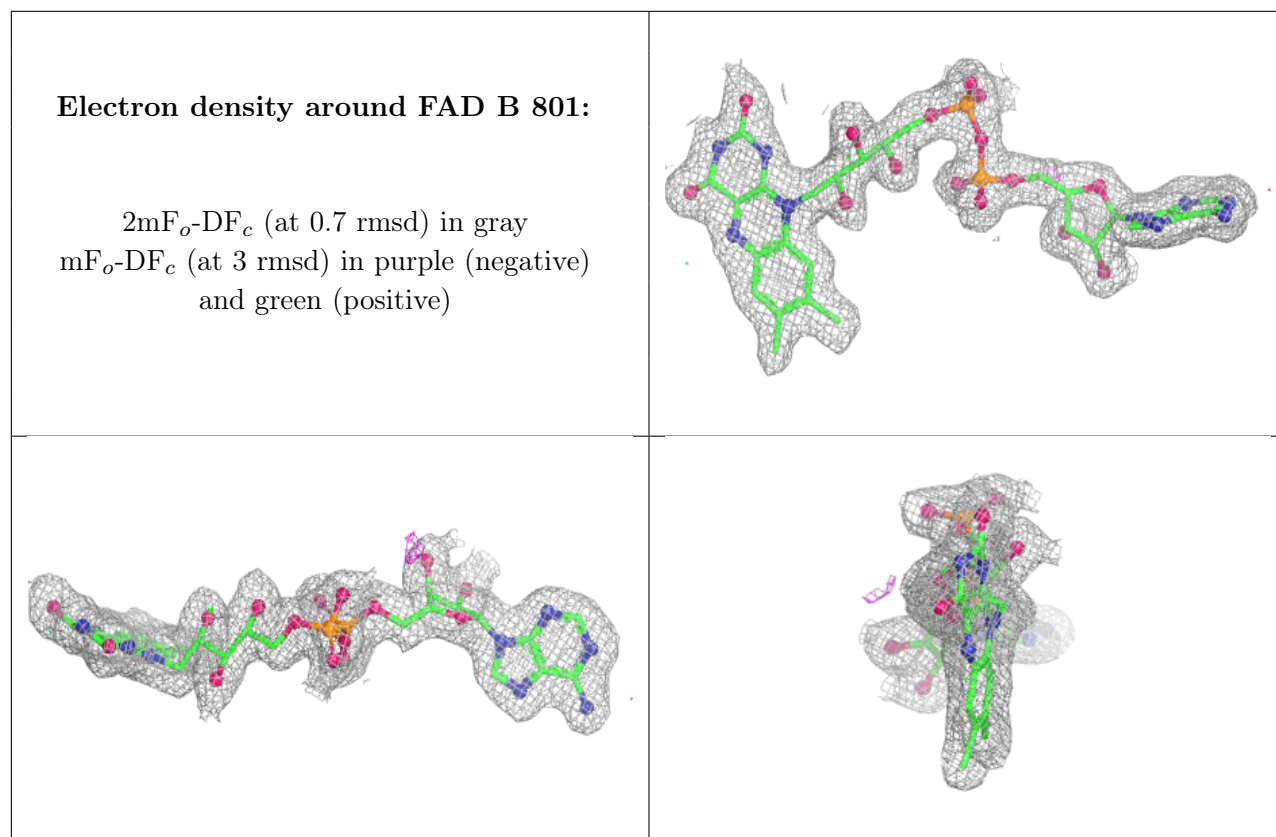
Electron density around FAD C 702:

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

**Electron density around FAD A 801:**

$2mF_o-DF_c$ (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.