



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:44 PM UTC

PDB ID : 5WX2 / pdb_00005wx2
Title : Crystal structure of porcine kidney D-amino acid oxidase mutant (I230A/R283G)
Authors : Motojima, F.; Yasukawa, K.; Ohno, A.; Asano, Y.
Deposited on : 2017-01-06
Resolution : 3.00 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)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

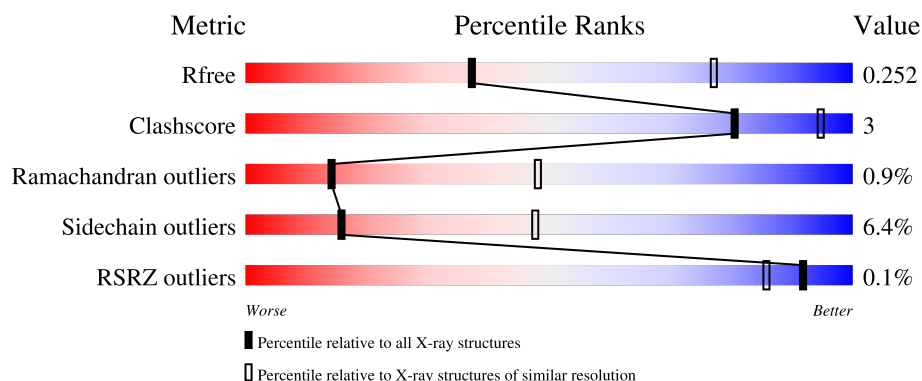
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	347	
1	B	347	
1	C	347	
1	D	347	
1	E	347	

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Mol	Chain	Length	Quality of chain
1	F	347	 86% 11% ..
1	G	347	 81% 15% ..
1	H	347	 82% 14% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22380 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 D-amino-acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	1	0
			2701	1737	469	486	9			
1	B	339	Total	C	N	O	S	0	0	0
			2710	1742	470	489	9			
1	C	339	Total	C	N	O	S	0	1	0
			2717	1747	472	489	9			
1	D	339	Total	C	N	O	S	0	0	0
			2710	1742	470	489	9			
1	E	339	Total	C	N	O	S	0	2	0
			2722	1750	473	490	9			
1	F	339	Total	C	N	O	S	0	0	0
			2710	1742	470	489	9			
1	G	338	Total	C	N	O	S	0	1	0
			2709	1741	471	488	9			
1	H	337	Total	C	N	O	S	0	1	0
			2701	1737	469	486	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	ALA	ILE	engineered mutation	UNP P00371
A	283	GLY	ARG	engineered mutation	UNP P00371
B	230	ALA	ILE	engineered mutation	UNP P00371
B	283	GLY	ARG	engineered mutation	UNP P00371
C	230	ALA	ILE	engineered mutation	UNP P00371
C	283	GLY	ARG	engineered mutation	UNP P00371
D	230	ALA	ILE	engineered mutation	UNP P00371
D	283	GLY	ARG	engineered mutation	UNP P00371
E	230	ALA	ILE	engineered mutation	UNP P00371
E	283	GLY	ARG	engineered mutation	UNP P00371
F	230	ALA	ILE	engineered mutation	UNP P00371
F	283	GLY	ARG	engineered mutation	UNP P00371
G	230	ALA	ILE	engineered mutation	UNP P00371

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Chain	Residue	Modelled	Actual	Comment	Reference
G	283	GLY	ARG	engineered mutation	UNP P00371
H	230	ALA	ILE	engineered mutation	UNP P00371
H	283	GLY	ARG	engineered mutation	UNP P00371

- # FAD

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $\text{C}_6\text{H}_{14}\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

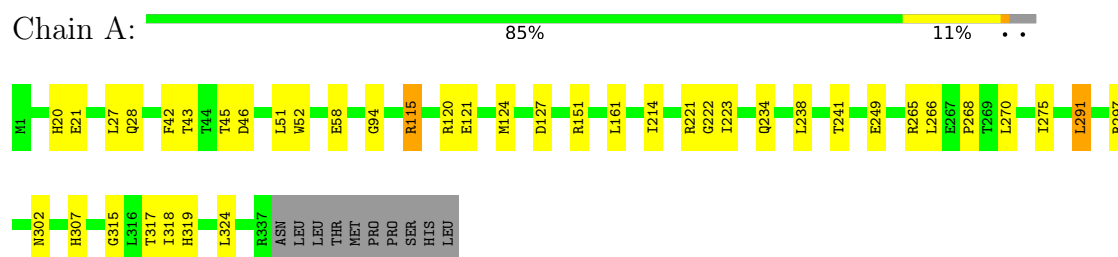
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		
5	B	22	Total	O	0	0
			22	22		
5	C	5	Total	O	0	0
			5	5		
5	D	10	Total	O	0	0
			10	10		
5	E	4	Total	O	0	0
			4	4		
5	F	2	Total	O	0	0
			2	2		
5	G	4	Total	O	0	0
			4	4		
5	H	5	Total	O	0	0
			5	5		

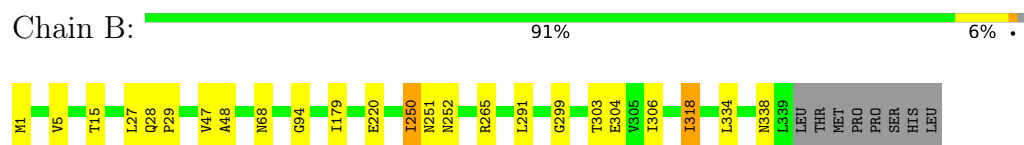
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

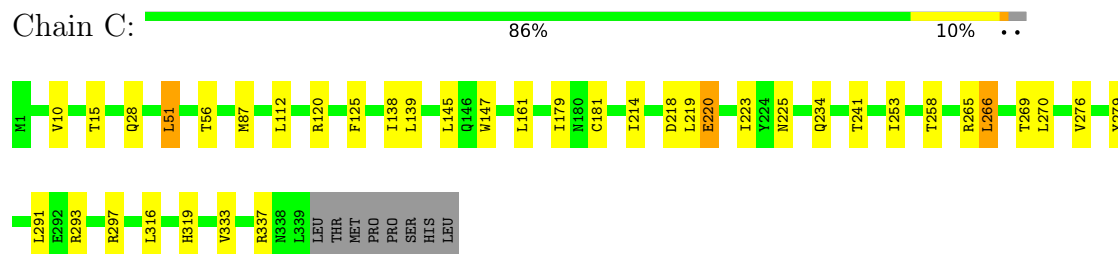
- Molecule 1: D-amino-acid oxidase



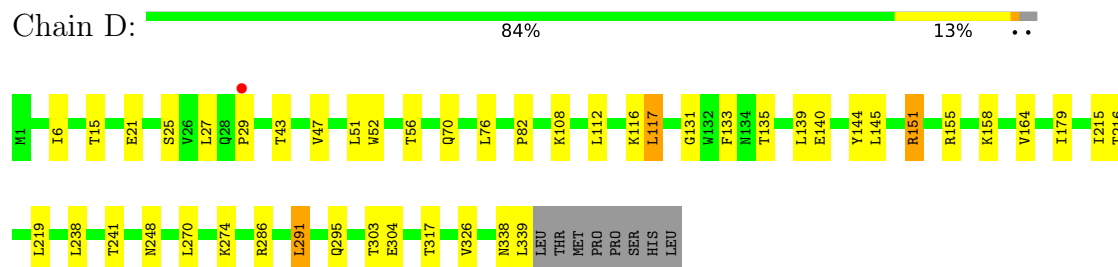
- Molecule 1: D-amino-acid oxidase



- Molecule 1: D-amino-acid oxidase

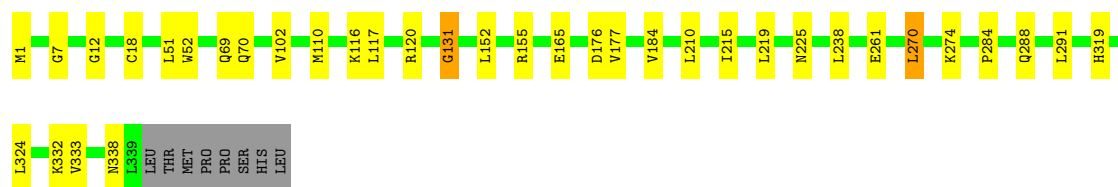


- Molecule 1: D-amino-acid oxidase



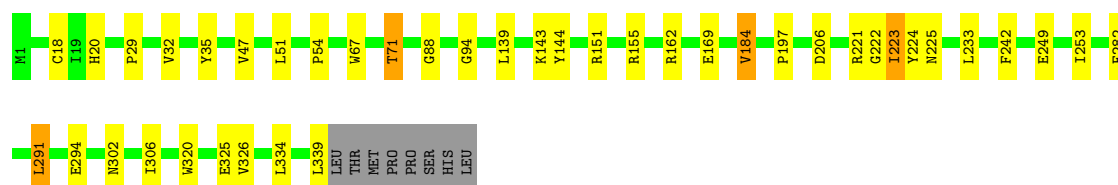
- Molecule 1: D-amino-acid oxidase

Chain E:  87% 10% ..



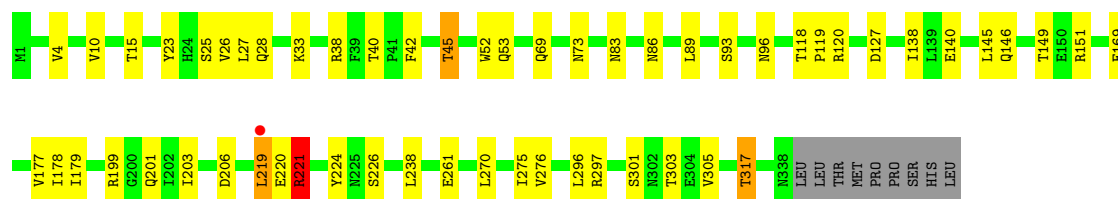
- Molecule 1: D-amino-acid oxidase

Chain F:  86% 11% ..



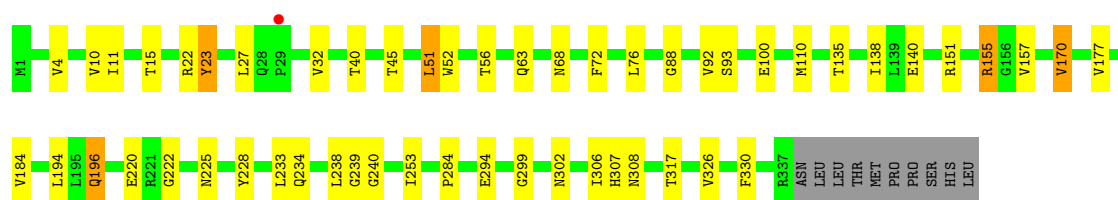
- Molecule 1: D-amino-acid oxidase

Chain G:  81% 15% ..



- Molecule 1: D-amino-acid oxidase

Chain H:  82% 14% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	168.40Å 270.90Å 135.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.17 – 3.00 49.17 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.17-3.00) 99.9 (49.17-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.165 , 0.253 0.171 , 0.252	Depositor DCC
R_{free} test set	2943 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22380	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FAD, MPD

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	0.82	0/2781	0.93	1/3788 (0.0%)
1	B	0.79	0/2786	0.93	1/3795 (0.0%)
1	C	0.72	0/2797	0.89	4/3810 (0.1%)
1	D	0.77	0/2786	0.90	1/3795 (0.0%)
1	E	0.73	0/2805	0.93	2/3821 (0.1%)
1	F	0.74	0/2786	0.91	1/3795 (0.0%)
1	G	0.70	0/2789	0.91	2/3799 (0.1%)
1	H	0.76	0/2781	0.90	2/3788 (0.1%)
All	All	0.76	0/22311	0.91	14/30391 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	94	GLY	N-CA-C	6.71	120.92	111.19
1	B	94	GLY	N-CA-C	6.51	119.35	110.69
1	H	56	THR	N-CA-C	5.65	119.43	112.54
1	C	56	THR	N-CA-C	5.58	117.36	111.28
1	H	23	TYR	N-CA-C	5.54	120.91	112.54
1	E	131	GLY	N-CA-C	5.36	118.36	110.80
1	G	301	SER	N-CA-C	5.33	122.16	110.80
1	D	131	GLY	N-CA-C	5.33	119.29	110.55
1	C	319	HIS	N-CA-C	5.28	117.72	111.33
1	A	94	GLY	N-CA-C	5.13	118.63	111.19
1	C	125	PHE	CA-C-N	5.08	126.19	119.84
1	C	125	PHE	C-N-CA	5.08	126.19	119.84
1	E	319	HIS	N-CA-C	5.06	117.45	111.33
1	G	23	TYR	N-CA-C	5.02	120.12	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2701	0	2649	12	0
1	B	2710	0	2659	11	0
1	C	2717	0	2666	12	0
1	D	2710	0	2659	11	0
1	E	2722	0	2672	15	1
1	F	2710	0	2659	9	1
1	G	2709	0	2655	22	0
1	H	2701	0	2649	22	1
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
2	E	53	0	31	0	0
2	F	53	0	31	0	0
2	G	53	0	31	0	0
2	H	53	0	31	0	0
3	A	32	0	56	2	0
3	B	32	0	56	0	0
3	C	8	0	14	2	0
3	D	24	0	42	0	0
3	E	8	0	14	0	0
3	F	32	0	56	0	0
3	G	24	0	42	2	0
3	H	16	0	28	0	0
4	A	5	0	0	1	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	E	5	0	0	1	0
4	F	5	0	0	0	0
4	H	5	0	0	0	0
5	A	18	0	0	0	0
5	B	22	0	0	1	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	4	0	0	0	0
5	F	2	0	0	0	0
5	G	4	0	0	0	0
5	H	5	0	0	0	2
All	All	22380	0	21824	113	4

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 3.

All (113) 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:27:LEU:HD13	1:D:339:LEU:HD11	1.73	0.69
1:A:46:ASP:HB3	3:A:403:MPD:H52	1.75	0.69
1:E:51:LEU:HD23	1:E:215:ILE:HD11	1.79	0.65
1:F:223:ILE:HG23	1:F:224:TYR:CE2	2.33	0.64
1:B:1:MET:HE3	1:B:334:LEU:HD23	1.81	0.61
1:H:52:TRP:CE2	1:H:317:THR:HG23	2.36	0.60
1:C:51:LEU:HD12	1:C:138:ILE:HD13	1.85	0.58
1:A:214:ILE:HG21	1:A:266:LEU:HD22	1.86	0.57
1:E:1:MET:HE1	1:E:177:VAL:HG23	1.87	0.57
1:A:115:ARG:NH2	1:A:121:GLU:OE2	2.38	0.57
1:C:293:ARG:NH1	1:C:333:VAL:HG22	2.20	0.56
1:H:4:VAL:HG11	1:H:170:VAL:HG13	1.87	0.56
1:E:51:LEU:CD2	1:E:215:ILE:HD11	2.36	0.56
1:C:218:ASP:O	1:C:220:GLU:N	2.39	0.56
1:G:52:TRP:HA	1:G:317:THR:HG22	1.88	0.55
1:B:68:ASN:ND2	1:B:318:ILE:HD12	2.21	0.55
1:G:296:LEU:HD12	1:G:305:VAL:HG21	1.88	0.55
1:H:92:VAL:HG11	1:H:138:ILE:HG13	1.89	0.55
1:C:15:THR:HG21	1:C:179:ILE:HG21	1.87	0.54
1:B:5:VAL:HG13	1:B:179:ILE:HB	1.89	0.54
1:A:291:LEU:HA	1:A:307:HIS:O	2.08	0.53
1:E:69:GLN:CA	1:E:110:MET:HE3	2.38	0.53
1:B:15:THR:HG21	1:B:179:ILE:HG21	1.90	0.53
1:G:238:LEU:HD21	1:G:270:LEU:HD13	1.90	0.53
1:E:120:ARG:NH1	4:E:403:SO4:O4	2.41	0.53
1:H:11:ILE:O	1:H:15:THR:HG23	2.09	0.53
1:H:10:VAL:HB	1:H:45:THR:HG21	1.90	0.52
1:H:177:VAL:HG11	1:H:330:PHE:HE1	1.74	0.52
1:F:67:TRP:O	1:F:71:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:LEU:HD11	1:F:144:TYR:CG	2.45	0.52
1:D:112:LEU:HB2	1:D:135:THR:HB	1.92	0.52
1:D:139:LEU:HD21	1:D:144:TYR:CE2	2.45	0.52
1:D:139:LEU:HD21	1:D:144:TYR:CD2	2.45	0.52
1:A:124:MET:HG2	5:B:521:HOH:O	2.10	0.51
1:E:210:LEU:HD11	1:E:270:LEU:HD13	1.93	0.51
1:B:28:GLN:N	1:B:29:PRO:HD3	2.26	0.51
1:G:69:GLN:HE21	1:G:73:ASN:HD21	1.58	0.51
1:A:120:ARG:HD3	4:A:406:SO4:S	2.51	0.51
1:E:52:TRP:HH2	1:E:110:MET:HE2	1.76	0.51
1:D:51:LEU:CD2	1:D:215:ILE:HD11	2.41	0.50
1:B:68:ASN:HD21	1:B:318:ILE:HD12	1.76	0.50
1:G:120:ARG:NH2	1:H:110:MET:O	2.45	0.50
1:C:279:TYR:CD1	3:C:402:MPD:H52	2.47	0.49
1:H:306:ILE:HG21	1:H:326:VAL:HG13	1.94	0.49
1:E:117:LEU:HD12	1:E:131:GLY:HA3	1.95	0.48
1:C:120:ARG:NH1	4:C:403:SO4:O3	2.38	0.48
1:F:184:VAL:HG21	1:F:282:PHE:O	2.13	0.48
1:H:72:PHE:HE1	1:H:76:LEU:HD12	1.79	0.47
1:E:69:GLN:HA	1:E:110:MET:HE3	1.95	0.47
1:B:28:GLN:N	1:B:29:PRO:CD	2.78	0.47
1:F:306:ILE:HG21	1:F:326:VAL:HG13	1.97	0.47
1:G:42:PHE:CZ	3:G:404:MPD:H51	2.49	0.46
1:G:10:VAL:HG12	1:G:45:THR:HG21	1.97	0.46
1:B:47:VAL:O	1:B:48:ALA:C	2.57	0.46
1:G:52:TRP:CD1	1:G:317:THR:HG22	2.50	0.46
1:H:68:ASN:ND2	1:H:317:THR:HG22	2.31	0.46
1:D:52:TRP:CD1	1:D:317:THR:HA	2.50	0.46
1:H:15:THR:HG21	1:H:308:ASN:HD22	1.81	0.46
1:A:42:PHE:HA	3:A:404:MPD:H12	1.98	0.46
1:C:179:ILE:HG22	1:C:181:CYS:SG	2.55	0.45
1:H:151:ARG:O	1:H:155:ARG:HG2	2.16	0.45
1:E:69:GLN:N	1:E:110:MET:HE3	2.31	0.45
1:G:15:THR:HG21	1:G:179:ILE:HG21	1.99	0.45
1:G:89:LEU:HA	1:G:138:ILE:O	2.17	0.45
1:B:1:MET:HE3	1:B:334:LEU:CD2	2.46	0.45
1:E:70:GLN:HE21	1:E:324:LEU:HD12	1.81	0.45
1:D:6:ILE:HD13	1:D:164:VAL:HG21	1.98	0.45
1:H:88:GLY:HA2	1:H:233:LEU:HD11	1.99	0.45
1:B:303:THR:HG22	1:B:304:GLU:N	2.32	0.44
1:C:214:ILE:HG21	1:C:266:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:VAL:HB	1:G:178:ILE:HG22	2.00	0.44
1:G:83:ASN:OD1	1:G:86:ASN:ND2	2.50	0.44
1:A:52:TRP:CE2	1:A:317:THR:HG23	2.53	0.44
1:H:294:GLU:OE1	1:H:307:HIS:NE2	2.46	0.44
1:C:87:MET:HG2	1:C:147:TRP:CD2	2.53	0.44
1:H:184:VAL:N	1:H:284:PRO:HB3	2.33	0.44
1:E:52:TRP:CH2	1:E:110:MET:HE2	2.53	0.43
1:F:88:GLY:HA2	1:F:233:LEU:HD11	2.00	0.43
1:C:225:ASN:HB3	1:C:258:THR:HG21	2.00	0.43
1:H:68:ASN:HD22	1:H:317:THR:HG22	1.83	0.43
1:G:53:GLN:HE22	1:G:96:ASN:HD21	1.67	0.43
1:C:279:TYR:CE1	3:C:402:MPD:H52	2.54	0.43
1:B:250:ILE:HG23	1:B:251:ASN:O	2.18	0.43
1:E:1:MET:HE3	1:E:176:ASP:HB2	2.01	0.43
1:H:93:SER:HA	1:H:135:THR:HA	2.00	0.43
1:A:20:HIS:CD2	1:A:20:HIS:C	2.97	0.43
1:G:118:THR:HB	1:G:119:PRO:HD2	2.01	0.43
1:G:53:GLN:NE2	1:G:96:ASN:OD1	2.52	0.43
1:G:151:ARG:NE	1:G:151:ARG:HA	2.34	0.43
1:G:53:GLN:H	1:G:317:THR:HG21	1.84	0.42
1:A:43:THR:OG1	1:A:45:THR:HB	2.19	0.42
1:G:52:TRP:HA	1:G:317:THR:CG2	2.47	0.42
1:A:151:ARG:NE	1:A:151:ARG:HA	2.35	0.42
1:A:315:GLY:O	1:A:319:HIS:HB3	2.20	0.42
1:F:71:THR:HG22	1:F:320:TRP:HB3	2.01	0.42
1:E:7:GLY:O	1:E:12:GLY:HA3	2.19	0.42
1:H:51:LEU:HD12	1:H:52:TRP:N	2.35	0.41
1:G:221:ARG:NE	1:G:221:ARG:HA	2.34	0.41
1:F:291:LEU:HD21	1:F:325:GLU:HB3	2.02	0.41
1:H:22:ARG:HG2	1:H:23:TYR:CE2	2.56	0.41
1:C:10:VAL:HG21	1:C:316:LEU:HD23	2.03	0.41
1:D:15:THR:HG21	1:D:179:ILE:HG21	2.02	0.41
1:D:151:ARG:O	1:D:155:ARG:HG2	2.21	0.41
1:H:32:VAL:HB	1:H:157:VAL:HG13	2.03	0.41
1:F:20:HIS:ND1	1:F:155:ARG:NH1	2.69	0.40
1:H:52:TRP:CZ2	1:H:72:PHE:HB2	2.56	0.40
1:E:184:VAL:N	1:E:284:PRO:HB3	2.35	0.40
1:D:117:LEU:CD1	1:D:133:PHE:HB2	2.51	0.40
1:G:199:ARG:NH2	1:G:201:GLN:OE1	2.55	0.40
1:G:203:ILE:HG23	1:G:275:ILE:HG23	2.04	0.40
1:H:228:TYR:CZ	1:H:239:GLY:HA3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:LEU:HD13	1:D:326:VAL:HG22	2.02	0.40
1:G:38:ARG:NH1	3:G:404:MPD:O2	2.55	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:503:HOH:O	5:H:503:HOH:O[4_556]	1.75	0.45
1:H:196:GLN:OE1	1:H:196:GLN:OE1[4_556]	2.10	0.10
5:H:502:HOH:O	5:H:502:HOH:O[4_556]	2.16	0.04
1:E:165:GLU:OE1	1:F:35:TYR:OH[6_544]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/347 (97%)	317 (94%)	17 (5%)	2 (1%)	21	56
1	B	337/347 (97%)	317 (94%)	19 (6%)	1 (0%)	36	70
1	C	338/347 (97%)	312 (92%)	25 (7%)	1 (0%)	36	70
1	D	337/347 (97%)	309 (92%)	25 (7%)	3 (1%)	14	48
1	E	339/347 (98%)	322 (95%)	14 (4%)	3 (1%)	14	48
1	F	337/347 (97%)	307 (91%)	24 (7%)	6 (2%)	6	31
1	G	337/347 (97%)	305 (90%)	30 (9%)	2 (1%)	21	56
1	H	336/347 (97%)	300 (89%)	30 (9%)	6 (2%)	6	31
All	All	2697/2776 (97%)	2489 (92%)	184 (7%)	24 (1%)	14	48

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	219	LEU
1	E	219	LEU
1	F	29	PRO
1	F	197	PRO
1	F	222	GLY
1	H	225	ASN
1	B	299	GLY
1	D	338	ASN
1	E	338	ASN
1	F	223	ILE
1	H	220	GLU
1	A	223	ILE
1	G	221	ARG
1	H	240	GLY
1	D	25	SER
1	E	225	ASN
1	F	221	ARG
1	G	219	LEU
1	H	222	GLY
1	H	100	GLU
1	D	29	PRO
1	F	54	PRO
1	H	299	GLY
1	A	222	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	287/296 (97%)	265 (92%)	22 (8%)	12	40
1	B	288/296 (97%)	279 (97%)	9 (3%)	35	68
1	C	289/296 (98%)	270 (93%)	19 (7%)	15	46
1	D	288/296 (97%)	262 (91%)	26 (9%)	9	34
1	E	290/296 (98%)	277 (96%)	13 (4%)	24	59
1	F	288/296 (97%)	268 (93%)	20 (7%)	14	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	288/296 (97%)	262 (91%)	26 (9%)	9	34
1	H	287/296 (97%)	274 (96%)	13 (4%)	24	59
All	All	2305/2368 (97%)	2157 (94%)	148 (6%)	16	48

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	27	LEU
1	A	28	GLN
1	A	51	LEU
1	A	58	GLU
1	A	115	ARG
1	A	127	ASP
1	A	161	LEU
1	A	221	ARG
1	A	234	GLN
1	A	238	LEU
1	A	241	THR
1	A	249	GLU
1	A	265	ARG
1	A	268	PRO
1	A	270	LEU
1	A	275	ILE
1	A	291	LEU
1	A	297	ARG
1	A	302	ASN
1	A	318	ILE
1	A	324	LEU
1	B	27	LEU
1	B	220	GLU
1	B	250	ILE
1	B	252	ASN
1	B	265	ARG
1	B	291	LEU
1	B	306	ILE
1	B	318	ILE
1	B	338	ASN
1	C	28	GLN
1	C	51	LEU
1	C	112	LEU

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Mol	Chain	Res	Type
1	C	139	LEU
1	C	145	LEU
1	C	161	LEU
1	C	220	GLU
1	C	223	ILE
1	C	234	GLN
1	C	241	THR
1	C	253	ILE
1	C	265	ARG
1	C	266	LEU
1	C	269	THR
1	C	270	LEU
1	C	276	VAL
1	C	291	LEU
1	C	297	ARG
1	C	337	ARG
1	D	21	GLU
1	D	43	THR
1	D	47	VAL
1	D	56	THR
1	D	70	GLN
1	D	76	LEU
1	D	82	PRO
1	D	108	LYS
1	D	116	LYS
1	D	117	LEU
1	D	140	GLU
1	D	145	LEU
1	D	151	ARG
1	D	158	LYS
1	D	216	THR
1	D	219	LEU
1	D	238	LEU
1	D	241	THR
1	D	248	ASN
1	D	270	LEU
1	D	274	LYS
1	D	286	ARG
1	D	291	LEU
1	D	295	GLN
1	D	303	THR
1	D	304	GLU

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Mol	Chain	Res	Type
1	E	18	CYS
1	E	102	VAL
1	E	116	LYS
1	E	152	LEU
1	E	155	ARG
1	E	238	LEU
1	E	261	GLU
1	E	270	LEU
1	E	274	LYS
1	E	288	GLN
1	E	291	LEU
1	E	332	LYS
1	E	333	VAL
1	F	18	CYS
1	F	32	VAL
1	F	47	VAL
1	F	51	LEU
1	F	71	THR
1	F	143	LYS
1	F	151	ARG
1	F	162	ARG
1	F	169	GLU
1	F	184	VAL
1	F	206	ASP
1	F	225	ASN
1	F	242	PHE
1	F	249	GLU
1	F	253	ILE
1	F	291	LEU
1	F	294	GLU
1	F	302	ASN
1	F	334	LEU
1	F	339	LEU
1	G	25	SER
1	G	26	VAL
1	G	27	LEU
1	G	28	GLN
1	G	33	LYS
1	G	40	THR
1	G	45	THR
1	G	93	SER
1	G	127	ASP

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Mol	Chain	Res	Type
1	G	140	GLU
1	G	145	LEU
1	G	146	GLN
1	G	149	THR
1	G	169	GLU
1	G	177	VAL
1	G	206	ASP
1	G	219	LEU
1	G	220	GLU
1	G	221	ARG
1	G	224	TYR
1	G	226	SER
1	G	261	GLU
1	G	276	VAL
1	G	297	ARG
1	G	303	THR
1	G	317	THR
1	H	27	LEU
1	H	40	THR
1	H	51	LEU
1	H	63	GLN
1	H	140	GLU
1	H	155	ARG
1	H	170	VAL
1	H	194	LEU
1	H	196	GLN
1	H	234	GLN
1	H	238	LEU
1	H	253	ILE
1	H	302	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	66	ASN
1	A	190	GLN
1	B	53	GLN
1	B	61	ASN
1	B	68	ASN
1	B	69	GLN
1	B	70	GLN

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Mol	Chain	Res	Type
1	B	73	ASN
1	B	96	ASN
1	B	180	ASN
1	B	190	GLN
1	B	234	GLN
1	C	68	ASN
1	C	69	GLN
1	C	134	ASN
1	C	248	ASN
1	C	302	ASN
1	D	63	GLN
1	D	68	ASN
1	D	70	GLN
1	D	83	ASN
1	D	86	ASN
1	D	96	ASN
1	D	196	GLN
1	D	212	ASN
1	D	234	GLN
1	D	254	GLN
1	D	288	GLN
1	E	20	HIS
1	E	68	ASN
1	E	69	GLN
1	E	70	GLN
1	E	251	ASN
1	F	66	ASN
1	F	69	GLN
1	F	70	GLN
1	F	83	ASN
1	F	86	ASN
1	F	243	GLN
1	F	248	ASN
1	F	257	ASN
1	G	53	GLN
1	G	68	ASN
1	G	69	GLN
1	G	70	GLN
1	G	83	ASN
1	G	86	ASN
1	G	96	ASN
1	G	134	ASN

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Mol	Chain	Res	Type
1	G	252	ASN
1	G	257	ASN
1	G	295	GLN
1	G	302	ASN
1	G	308	ASN
1	H	63	GLN
1	H	68	ASN
1	H	78	HIS
1	H	180	ASN
1	H	248	ASN
1	H	302	ASN
1	H	308	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](#)

36 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	MPD	D	404	-	7,7,7	0.39	0	9,10,10	0.61	0
2	FAD	C	401	-	58,58,58	1.63	11 (18%)	85,89,89	1.58	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MPD	B	403	-	7,7,7	0.35	0	9,10,10	0.42	0
2	FAD	F	401	-	58,58,58	1.62	12 (20%)	85,89,89	1.55	17 (20%)
4	SO4	F	406	-	4,4,4	0.47	0	6,6,6	0.29	0
2	FAD	E	401	-	58,58,58	1.47	10 (17%)	85,89,89	1.70	19 (22%)
4	SO4	A	406	-	4,4,4	0.50	0	6,6,6	0.42	0
2	FAD	D	401	-	58,58,58	1.57	11 (18%)	85,89,89	1.70	22 (25%)
2	FAD	B	401	-	58,58,58	1.48	10 (17%)	85,89,89	1.61	14 (16%)
3	MPD	E	402	-	7,7,7	0.31	0	9,10,10	0.34	0
3	MPD	H	403	-	7,7,7	0.35	0	9,10,10	0.77	0
4	SO4	H	404	-	4,4,4	0.47	0	6,6,6	0.34	0
3	MPD	G	403	-	7,7,7	0.33	0	9,10,10	0.35	0
3	MPD	B	405	-	7,7,7	0.41	0	9,10,10	0.42	0
3	MPD	D	403	-	7,7,7	0.39	0	9,10,10	0.60	0
3	MPD	F	404	-	7,7,7	0.29	0	9,10,10	0.32	0
3	MPD	B	402	-	7,7,7	0.22	0	9,10,10	0.84	0
2	FAD	G	401	-	58,58,58	1.61	11 (18%)	85,89,89	1.57	17 (20%)
3	MPD	B	404	-	7,7,7	0.42	0	9,10,10	0.37	0
4	SO4	D	405	-	4,4,4	0.45	0	6,6,6	0.36	0
3	MPD	G	404	-	7,7,7	0.37	0	9,10,10	0.67	0
3	MPD	C	402	-	7,7,7	0.50	0	9,10,10	0.63	0
3	MPD	F	405	-	7,7,7	0.39	0	9,10,10	0.42	0
3	MPD	H	402	-	7,7,7	0.28	0	9,10,10	0.52	0
4	SO4	E	403	-	4,4,4	0.52	0	6,6,6	0.29	0
3	MPD	A	405	-	7,7,7	0.55	0	9,10,10	0.76	0
3	MPD	D	402	-	7,7,7	0.28	0	9,10,10	0.69	0
3	MPD	G	402	-	7,7,7	0.34	0	9,10,10	0.24	0
3	MPD	F	403	-	7,7,7	0.47	0	9,10,10	0.58	0
2	FAD	A	401	-	58,58,58	1.56	12 (20%)	85,89,89	1.70	16 (18%)
3	MPD	A	402	-	7,7,7	0.34	0	9,10,10	0.66	0
2	FAD	H	401	-	58,58,58	1.41	9 (15%)	85,89,89	1.70	16 (18%)
3	MPD	A	403	-	7,7,7	0.25	0	9,10,10	0.60	0
4	SO4	C	403	-	4,4,4	0.45	0	6,6,6	0.61	0
3	MPD	F	402	-	7,7,7	0.30	0	9,10,10	0.40	0
3	MPD	A	404	-	7,7,7	0.46	0	9,10,10	1.08	1 (11%)

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	MPD	D	404	-	-	1/5/5/5	-
2	FAD	C	401	-	-	4/34/50/50	0/6/6/6
3	MPD	B	403	-	-	0/5/5/5	-
2	FAD	F	401	-	-	0/34/50/50	0/6/6/6
2	FAD	E	401	-	-	1/34/50/50	0/6/6/6
2	FAD	D	401	-	-	0/34/50/50	0/6/6/6
2	FAD	B	401	-	-	3/34/50/50	0/6/6/6
3	MPD	E	402	-	-	0/5/5/5	-
3	MPD	H	403	-	-	2/5/5/5	-
3	MPD	G	403	-	-	2/5/5/5	-
3	MPD	B	405	-	-	3/5/5/5	-
3	MPD	D	403	-	-	3/5/5/5	-
3	MPD	F	404	-	-	4/5/5/5	-
3	MPD	B	402	-	-	2/5/5/5	-
2	FAD	G	401	-	-	0/34/50/50	0/6/6/6
3	MPD	B	404	-	-	0/5/5/5	-
3	MPD	G	404	-	-	2/5/5/5	-
3	MPD	C	402	-	-	0/5/5/5	-
3	MPD	F	405	-	-	1/5/5/5	-
3	MPD	H	402	-	-	1/5/5/5	-
3	MPD	A	405	-	-	3/5/5/5	-
3	MPD	D	402	-	-	1/5/5/5	-
3	MPD	G	402	-	-	4/5/5/5	-
3	MPD	F	403	-	-	3/5/5/5	-
2	FAD	A	401	-	-	3/34/50/50	0/6/6/6
3	MPD	A	402	-	-	2/5/5/5	-
2	FAD	H	401	-	-	5/34/50/50	0/6/6/6
3	MPD	A	403	-	-	3/5/5/5	-
3	MPD	F	402	-	-	0/5/5/5	-
3	MPD	A	404	-	-	1/5/5/5	-

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FAD	C9A-C5X	6.09	1.51	1.41
2	F	401	FAD	C9A-C5X	5.95	1.50	1.41
2	A	401	FAD	C9A-C5X	5.72	1.50	1.41
2	G	401	FAD	C9A-C5X	5.62	1.50	1.41
2	E	401	FAD	C9A-C5X	5.08	1.49	1.41
2	D	401	FAD	C9A-C5X	5.07	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	FAD	C5A-C4A	5.04	1.48	1.39
2	G	401	FAD	C5A-C4A	5.02	1.48	1.39
2	C	401	FAD	C5A-C4A	4.99	1.48	1.39
2	B	401	FAD	C9A-C5X	4.99	1.49	1.41
2	H	401	FAD	C9A-C5X	4.69	1.48	1.41
2	F	401	FAD	C5A-C4A	4.58	1.47	1.39
2	A	401	FAD	C5A-C4A	4.27	1.46	1.39
2	C	401	FAD	C8-C7	4.10	1.50	1.40
2	H	401	FAD	C5A-C4A	3.96	1.46	1.39
2	D	401	FAD	P-O3P	3.91	1.63	1.59
2	B	401	FAD	C5A-C4A	3.84	1.45	1.39
2	E	401	FAD	C5A-C4A	3.79	1.45	1.39
2	F	401	FAD	PA-O3P	3.68	1.63	1.59
2	E	401	FAD	C8-C7	3.54	1.49	1.40
2	G	401	FAD	C8-C7	3.41	1.49	1.40
2	G	401	FAD	PA-O3P	3.32	1.63	1.59
2	E	401	FAD	P-O3P	3.21	1.63	1.59
2	F	401	FAD	C8-C7	3.19	1.48	1.40
2	A	401	FAD	C8-C7	3.17	1.48	1.40
2	H	401	FAD	C8-C7	3.15	1.48	1.40
2	B	401	FAD	C5A-N7A	-3.14	1.33	1.39
2	F	401	FAD	P-O3P	3.00	1.62	1.59
2	H	401	FAD	C5A-N7A	-2.98	1.33	1.39
2	C	401	FAD	C5A-C6A	2.95	1.49	1.41
2	D	401	FAD	C8-C7	2.88	1.47	1.40
2	A	401	FAD	C5A-C6A	2.86	1.49	1.41
2	B	401	FAD	C8-C7	2.85	1.47	1.40
2	G	401	FAD	C4A-N9A	-2.78	1.31	1.37
2	E	401	FAD	C5A-C6A	2.78	1.48	1.41
2	D	401	FAD	C5A-C6A	2.78	1.48	1.41
2	B	401	FAD	C4A-N9A	-2.76	1.32	1.37
2	F	401	FAD	C8A-N7A	2.72	1.36	1.31
2	G	401	FAD	C8A-N7A	2.70	1.36	1.31
2	D	401	FAD	C8A-N7A	2.70	1.36	1.31
2	C	401	FAD	C5X-N5	-2.59	1.34	1.39
2	H	401	FAD	C5X-N5	-2.49	1.34	1.39
2	F	401	FAD	C5X-N5	-2.48	1.34	1.39
2	F	401	FAD	C4A-N9A	-2.48	1.32	1.37
2	B	401	FAD	PA-O3P	2.44	1.62	1.59
2	A	401	FAD	C4-N3	-2.43	1.34	1.38
2	E	401	FAD	C4A-N9A	-2.41	1.32	1.37
2	C	401	FAD	P-O3P	2.40	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	FAD	C5A-N7A	-2.38	1.34	1.39
2	C	401	FAD	C4-N3	-2.38	1.34	1.38
2	G	401	FAD	C5A-C6A	2.37	1.47	1.41
2	A	401	FAD	P-O3P	2.36	1.62	1.59
2	G	401	FAD	P-O3P	2.36	1.62	1.59
2	B	401	FAD	C5A-C6A	2.35	1.47	1.41
2	B	401	FAD	P-O3P	2.34	1.62	1.59
2	G	401	FAD	C5A-N7A	-2.32	1.34	1.39
2	D	401	FAD	C5A-N7A	-2.30	1.34	1.39
2	D	401	FAD	PA-O3P	2.30	1.62	1.59
2	A	401	FAD	PA-O3P	2.30	1.62	1.59
2	C	401	FAD	C8A-N7A	2.29	1.36	1.31
2	F	401	FAD	C5A-C6A	2.28	1.47	1.41
2	A	401	FAD	C8A-N7A	2.28	1.36	1.31
2	C	401	FAD	C4A-N9A	-2.27	1.33	1.37
2	D	401	FAD	C4A-N9A	-2.26	1.33	1.37
2	B	401	FAD	C5X-N5	-2.25	1.35	1.39
2	G	401	FAD	C4-N3	-2.23	1.34	1.38
2	B	401	FAD	C4-N3	-2.22	1.34	1.38
2	F	401	FAD	C10-N10	2.21	1.42	1.37
2	D	401	FAD	C10-N10	2.21	1.42	1.37
2	F	401	FAD	C4-N3	-2.20	1.34	1.38
2	E	401	FAD	PA-O3P	2.20	1.61	1.59
2	H	401	FAD	C8A-N7A	2.19	1.35	1.31
2	E	401	FAD	C5A-N7A	-2.17	1.35	1.39
2	H	401	FAD	C4A-N9A	-2.15	1.33	1.37
2	H	401	FAD	C4-N3	-2.14	1.34	1.38
2	H	401	FAD	C5A-C6A	2.14	1.46	1.41
2	A	401	FAD	C5X-N5	-2.13	1.35	1.39
2	C	401	FAD	C5A-N7A	-2.12	1.35	1.39
2	C	401	FAD	C10-N10	2.09	1.41	1.37
2	G	401	FAD	C4X-N5	2.08	1.35	1.30
2	A	401	FAD	C5A-N7A	-2.08	1.35	1.39
2	A	401	FAD	C4A-N9A	-2.07	1.33	1.37
2	E	401	FAD	C8A-N7A	2.06	1.35	1.31
2	E	401	FAD	C5X-N5	-2.06	1.35	1.39
2	D	401	FAD	C4-N3	-2.03	1.35	1.38
2	A	401	FAD	C2-N3	-2.02	1.34	1.39

All (140) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FAD	C5A-C4A-N3A	-6.72	117.47	126.72
2	H	401	FAD	C5A-C4A-N3A	-6.14	118.26	126.72
2	D	401	FAD	C5A-C4A-N3A	-5.75	118.81	126.72
2	B	401	FAD	C5A-C4A-N3A	-5.34	119.37	126.72
2	E	401	FAD	C5A-C4A-N3A	-5.07	119.74	126.72
2	H	401	FAD	N3A-C4A-N9A	5.06	135.77	127.17
2	C	401	FAD	C5A-C4A-N3A	-4.99	119.85	126.72
2	A	401	FAD	N3A-C4A-N9A	4.92	135.54	127.17
2	G	401	FAD	C5A-C4A-N3A	-4.77	120.15	126.72
2	F	401	FAD	C5A-C4A-N3A	-4.66	120.31	126.72
2	A	401	FAD	C2A-N3A-C4A	4.48	122.78	111.83
2	E	401	FAD	N3A-C2A-N1A	-4.36	121.98	128.58
2	C	401	FAD	N3A-C4A-N9A	4.15	134.22	127.17
2	E	401	FAD	C2A-N3A-C4A	4.04	121.69	111.83
2	D	401	FAD	N3A-C4A-N9A	3.98	133.94	127.17
2	E	401	FAD	N3A-C4A-N9A	3.98	133.94	127.17
2	F	401	FAD	N3A-C4A-N9A	3.94	133.88	127.17
2	H	401	FAD	C2A-N3A-C4A	3.91	121.38	111.83
2	H	401	FAD	N3A-C2A-N1A	-3.88	122.72	128.58
2	B	401	FAD	C2A-N3A-C4A	3.86	121.25	111.83
2	G	401	FAD	C4-C4X-N5	3.85	123.53	118.21
2	D	401	FAD	C2A-N3A-C4A	3.84	121.20	111.83
2	B	401	FAD	N3A-C2A-N1A	-3.82	122.80	128.58
2	G	401	FAD	N3A-C4A-N9A	3.69	133.45	127.17
2	G	401	FAD	N3A-C2A-N1A	-3.67	123.03	128.58
2	B	401	FAD	N3A-C4A-N9A	3.67	133.40	127.17
2	C	401	FAD	O4-C4-C4X	-3.61	117.00	126.53
2	B	401	FAD	C4A-C5A-N7A	-3.60	106.47	110.58
2	A	401	FAD	N3A-C2A-N1A	-3.58	123.16	128.58
2	D	401	FAD	C4A-C5A-N7A	-3.57	106.50	110.58
2	F	401	FAD	N3A-C2A-N1A	-3.55	123.21	128.58
2	D	401	FAD	C4-C4X-N5	3.48	123.02	118.21
2	F	401	FAD	C2A-N3A-C4A	3.46	120.28	111.83
2	B	401	FAD	O4B-C1B-N9A	3.46	114.73	108.09
2	G	401	FAD	C2A-N3A-C4A	3.40	120.14	111.83
2	D	401	FAD	N3A-C2A-N1A	-3.37	123.48	128.58
2	F	401	FAD	C4A-N9A-C8A	3.33	109.23	105.74
2	C	401	FAD	C2A-N3A-C4A	3.32	119.93	111.83
2	H	401	FAD	C4A-C5A-N7A	-3.31	106.80	110.58
2	E	401	FAD	O4-C4-C4X	-3.27	117.89	126.53
2	H	401	FAD	C4A-N9A-C8A	3.24	109.14	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FAD	C4A-C5A-N7A	-3.22	106.91	110.58
2	E	401	FAD	C4A-C5A-N7A	-3.21	106.91	110.58
2	F	401	FAD	C4X-C10-N1	-3.18	116.79	124.59
2	H	401	FAD	O2-C2-N1	-3.17	116.53	121.80
2	D	401	FAD	C10-N1-C2	3.16	123.68	116.85
2	A	401	FAD	C4A-C5A-N7A	-3.08	107.06	110.58
2	E	401	FAD	C4A-N9A-C8A	3.07	108.96	105.74
2	B	401	FAD	O4-C4-C4X	-3.06	118.45	126.53
2	D	401	FAD	C4X-C10-N1	-3.05	117.11	124.59
2	C	401	FAD	C4X-C10-N1	-3.04	117.14	124.59
2	C	401	FAD	N3A-C2A-N1A	-3.01	124.03	128.58
2	D	401	FAD	O3'-C3'-C2'	2.98	115.71	108.93
2	E	401	FAD	C4X-C10-N1	-2.94	117.38	124.59
2	B	401	FAD	C4X-C10-N1	-2.89	117.51	124.59
2	D	401	FAD	C2B-C1B-N9A	2.87	120.44	113.30
2	E	401	FAD	O2-C2-N1	-2.87	117.04	121.80
2	C	401	FAD	C9A-C5X-N5	-2.84	119.44	122.45
2	C	401	FAD	C4A-N9A-C8A	2.83	108.71	105.74
2	G	401	FAD	O4B-C1B-N9A	2.83	113.53	108.09
2	H	401	FAD	C5A-N7A-C8A	2.80	107.86	103.45
2	E	401	FAD	C6A-C5A-N7A	2.78	137.46	132.09
2	A	401	FAD	C4X-C10-N1	-2.76	117.81	124.59
2	H	401	FAD	N9A-C8A-N7A	-2.70	110.10	113.94
2	G	401	FAD	C4X-C4-N3	2.70	120.13	113.25
2	C	401	FAD	C4-N3-C2	-2.70	120.84	125.64
2	G	401	FAD	C10-N1-C2	2.70	122.69	116.85
2	H	401	FAD	O3P-P-O1P	-2.68	102.64	110.70
2	F	401	FAD	O4-C4-C4X	-2.68	119.45	126.53
2	F	401	FAD	C10-N1-C2	2.68	122.65	116.85
2	E	401	FAD	C10-N1-C2	2.68	122.64	116.85
2	F	401	FAD	C4X-C10-N10	2.65	120.28	116.48
2	A	401	FAD	O4B-C1B-C2B	-2.65	100.94	106.62
2	A	401	FAD	C4-C4X-N5	2.62	121.82	118.21
2	D	401	FAD	C4X-C4-N3	2.60	119.86	113.25
2	C	401	FAD	C4X-C4-N3	2.58	119.82	113.25
2	D	401	FAD	O4B-C1B-C2B	-2.56	101.13	106.62
2	B	401	FAD	C5A-N7A-C8A	2.56	107.48	103.45
2	F	401	FAD	C4A-C5A-N7A	-2.56	107.66	110.58
2	E	401	FAD	C4-N3-C2	-2.54	121.12	125.64
2	A	401	FAD	C2B-C1B-N9A	2.54	119.62	113.30
2	H	401	FAD	O4-C4-C4X	-2.54	119.83	126.53
2	B	401	FAD	C10-N1-C2	2.53	122.32	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	FAD	C4X-C10-N1	-2.52	118.42	124.59
2	B	401	FAD	C4X-C4-N3	2.51	119.65	113.25
2	D	401	FAD	C4X-C10-N10	2.50	120.06	116.48
2	G	401	FAD	C4A-C5A-N7A	-2.49	107.73	110.58
2	B	401	FAD	C6A-C5A-N7A	2.45	136.81	132.09
2	C	401	FAD	C6-C5X-C9A	2.45	122.41	119.05
2	E	401	FAD	N9A-C8A-N7A	-2.44	110.47	113.94
2	D	401	FAD	C4'-C3'-C2'	-2.44	109.51	113.57
2	G	401	FAD	C2A-N1A-C6A	2.43	122.72	118.73
2	C	401	FAD	C5X-N5-C4X	2.43	122.01	118.09
2	E	401	FAD	C4X-C10-N10	2.42	119.94	116.48
2	E	401	FAD	C4-C4X-N5	2.40	121.52	118.21
2	E	401	FAD	C5A-N7A-C8A	2.37	107.18	103.45
2	H	401	FAD	O2P-P-O3P	2.37	113.68	107.27
2	C	401	FAD	N6A-C6A-N1A	2.36	123.63	118.38
2	D	401	FAD	O2P-P-O3P	2.35	113.64	107.27
2	G	401	FAD	C4X-C10-N1	-2.34	118.86	124.59
2	F	401	FAD	N9A-C8A-N7A	-2.34	110.62	113.94
2	A	401	FAD	C6A-C5A-N7A	2.33	136.58	132.09
2	F	401	FAD	C4-N3-C2	-2.33	121.51	125.64
2	C	401	FAD	C10-N1-C2	2.31	121.84	116.85
2	G	401	FAD	C5'-C4'-C3'	2.30	116.56	112.22
2	D	401	FAD	C4-N3-C2	-2.30	121.56	125.64
2	B	401	FAD	C4-N3-C2	-2.29	121.57	125.64
2	C	401	FAD	N10-C10-N1	2.29	125.25	118.51
2	A	401	FAD	C4X-C10-N10	2.28	119.75	116.48
2	G	401	FAD	O4-C4-C4X	-2.27	120.53	126.53
2	E	401	FAD	C4X-C4-N3	2.27	119.04	113.25
2	A	401	FAD	C5X-N5-C4X	2.26	121.74	118.09
2	D	401	FAD	O2A-PA-O1A	2.25	122.92	112.44
2	H	401	FAD	C4X-C10-N10	2.24	119.69	116.48
2	G	401	FAD	C4A-N9A-C8A	2.23	108.08	105.74
2	F	401	FAD	C9A-N10-C10	-2.22	117.36	120.75
2	C	401	FAD	C2A-N1A-C6A	2.21	122.37	118.73
2	G	401	FAD	O2A-PA-O1A	2.21	122.72	112.44
2	D	401	FAD	C10-C4X-N5	-2.20	120.31	124.81
2	D	401	FAD	C6A-C5A-N7A	2.20	136.33	132.09
2	F	401	FAD	O2-C2-N1	-2.20	118.15	121.80
2	H	401	FAD	C5X-N5-C4X	2.17	121.60	118.09
2	G	401	FAD	O2A-PA-O3P	-2.17	101.42	107.27
2	E	401	FAD	C9-C9A-N10	2.14	124.74	121.85
2	A	401	FAD	C5A-N7A-C8A	2.13	106.80	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	FAD	C4X-C10-N10	2.13	119.54	116.48
2	C	401	FAD	C5A-N7A-C8A	2.13	106.80	103.45
2	D	401	FAD	O4-C4-C4X	-2.12	120.94	126.53
2	D	401	FAD	C5A-N7A-C8A	2.10	106.75	103.45
2	F	401	FAD	O4B-C1B-N9A	2.10	112.11	108.09
2	B	401	FAD	N9A-C8A-N7A	-2.09	110.96	113.94
2	H	401	FAD	C4-N3-C2	-2.09	121.93	125.64
2	A	401	FAD	C10-N1-C2	2.08	121.35	116.85
2	E	401	FAD	C4A-N9A-C1B	-2.06	121.81	126.63
2	D	401	FAD	C5X-N5-C4X	2.04	121.39	118.09
3	A	404	MPD	CM-C2-C1	-2.03	106.08	110.63
2	A	401	FAD	C10-C4X-N5	-2.03	120.66	124.81
2	F	401	FAD	C5A-N7A-C8A	2.02	106.62	103.45
2	F	401	FAD	C4X-C4-N3	2.01	118.36	113.25
2	A	401	FAD	C4'-C3'-C2'	-2.00	110.24	113.57

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	401	FAD	C5'-O5'-P-O1P
2	H	401	FAD	C5'-O5'-P-O3P
3	A	402	MPD	C2-C3-C4-O4
3	A	402	MPD	C2-C3-C4-C5
3	A	403	MPD	C2-C3-C4-C5
3	D	403	MPD	C1-C2-C3-C4
3	D	403	MPD	O2-C2-C3-C4
3	F	403	MPD	C1-C2-C3-C4
3	F	403	MPD	O2-C2-C3-C4
3	G	404	MPD	C2-C3-C4-O4
3	G	404	MPD	C2-C3-C4-C5
2	A	401	FAD	P-O3P-PA-O5B
2	H	401	FAD	P-O3P-PA-O5B
2	B	401	FAD	O4B-C4B-C5B-O5B
2	B	401	FAD	C3B-C4B-C5B-O5B
2	H	401	FAD	PA-O3P-P-O2P
3	A	403	MPD	CM-C2-C3-C4
3	A	405	MPD	C1-C2-C3-C4
3	B	402	MPD	C1-C2-C3-C4
3	B	405	MPD	C1-C2-C3-C4
3	B	405	MPD	CM-C2-C3-C4
3	F	404	MPD	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	G	402	MPD	C1-C2-C3-C4
2	B	401	FAD	C5'-O5'-P-O1P
2	C	401	FAD	C5'-O5'-P-O1P
3	A	405	MPD	C2-C3-C4-C5
3	G	403	MPD	C2-C3-C4-C5
2	H	401	FAD	PA-O3P-P-O1P
2	A	401	FAD	PA-O3P-P-O2P
2	C	401	FAD	PA-O3P-P-O2P
2	C	401	FAD	O4B-C4B-C5B-O5B
2	A	401	FAD	O4B-C4B-C5B-O5B
3	B	405	MPD	O2-C2-C3-C4
3	F	404	MPD	O2-C2-C3-C4
3	G	402	MPD	O2-C2-C3-C4
3	H	402	MPD	O2-C2-C3-C4
3	D	402	MPD	C2-C3-C4-O4
3	F	404	MPD	C2-C3-C4-O4
3	G	402	MPD	C2-C3-C4-O4
3	G	403	MPD	C2-C3-C4-O4
3	A	403	MPD	C1-C2-C3-C4
3	A	404	MPD	C1-C2-C3-C4
3	A	405	MPD	CM-C2-C3-C4
3	B	402	MPD	CM-C2-C3-C4
3	D	403	MPD	CM-C2-C3-C4
3	D	404	MPD	C1-C2-C3-C4
3	F	403	MPD	CM-C2-C3-C4
3	F	404	MPD	CM-C2-C3-C4
3	F	405	MPD	C1-C2-C3-C4
3	G	402	MPD	CM-C2-C3-C4
3	H	403	MPD	C1-C2-C3-C4
3	H	403	MPD	CM-C2-C3-C4
2	E	401	FAD	O4B-C4B-C5B-O5B
2	C	401	FAD	PA-O3P-P-O1P

There are no ring outliers.

7 monomers are involved in 9 short contacts:

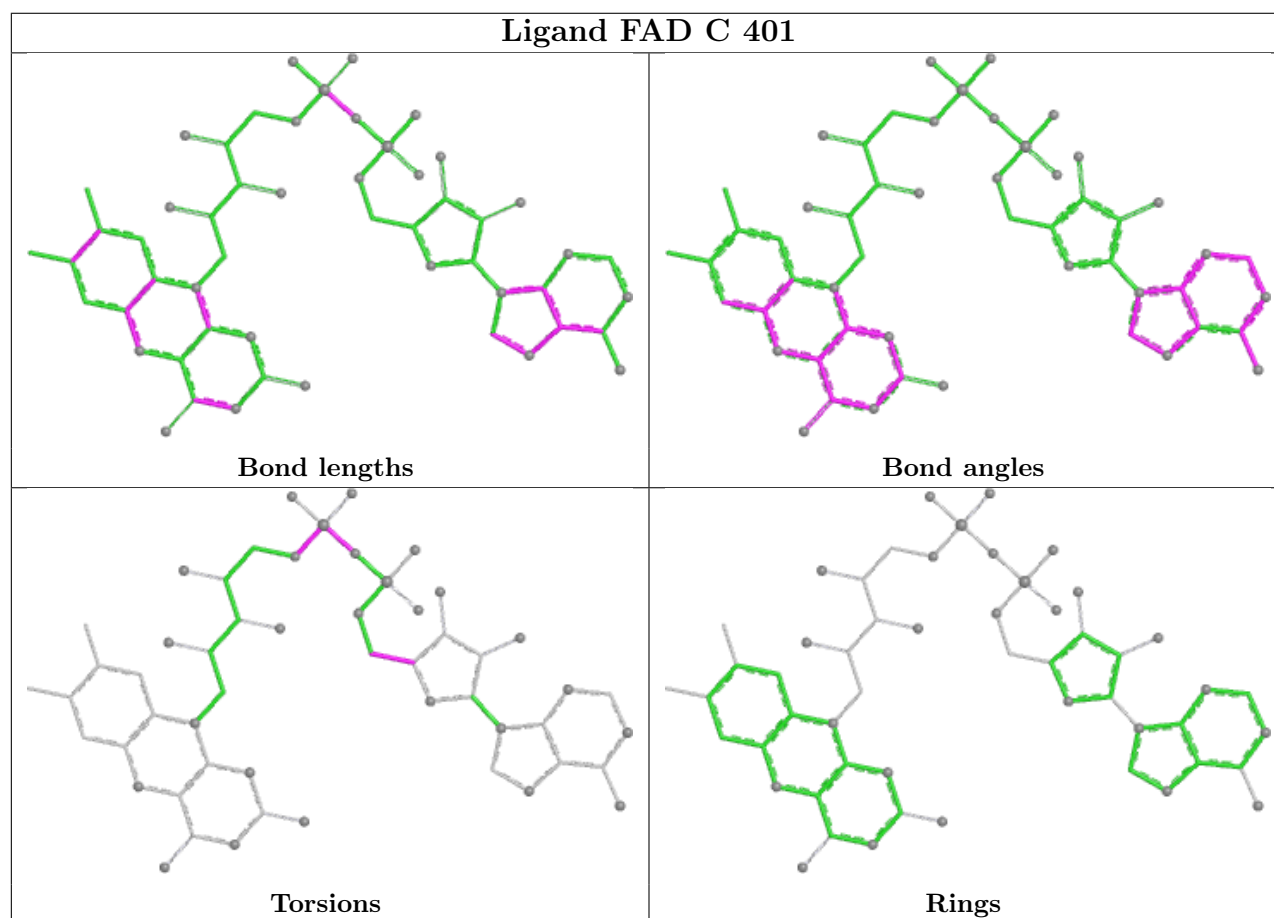
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	406	SO4	1	0
3	G	404	MPD	2	0
3	C	402	MPD	2	0
4	E	403	SO4	1	0
3	A	403	MPD	1	0

Continued on next page...

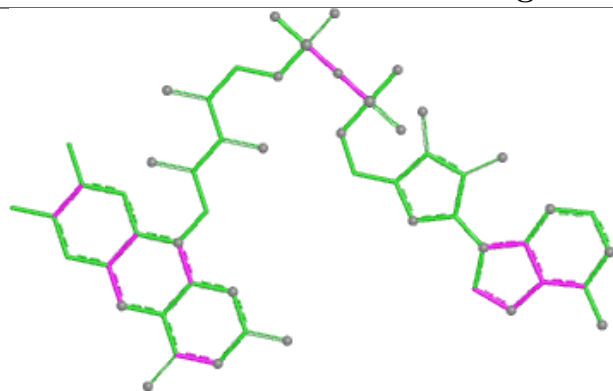
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	SO4	1	0
3	A	404	MPD	1	0

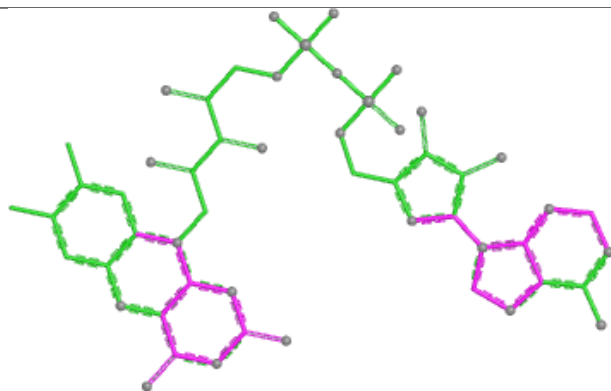
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



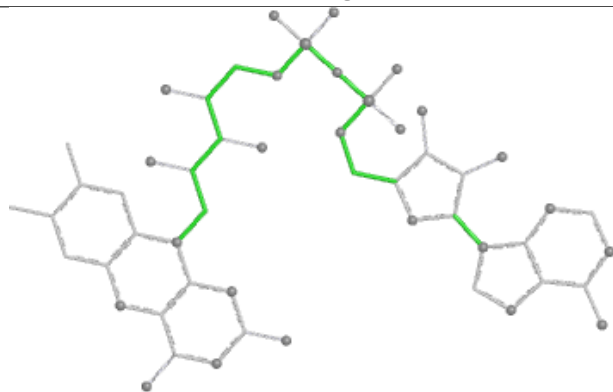
Ligand FAD F 401



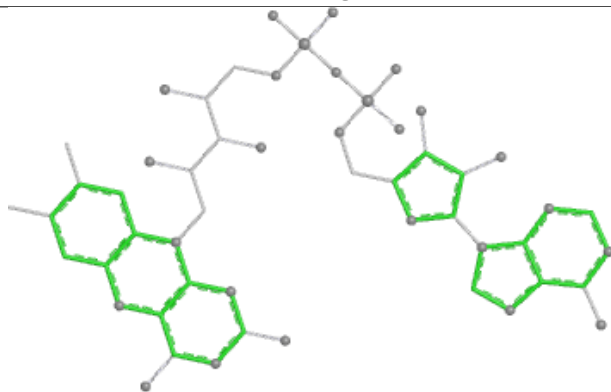
Bond lengths



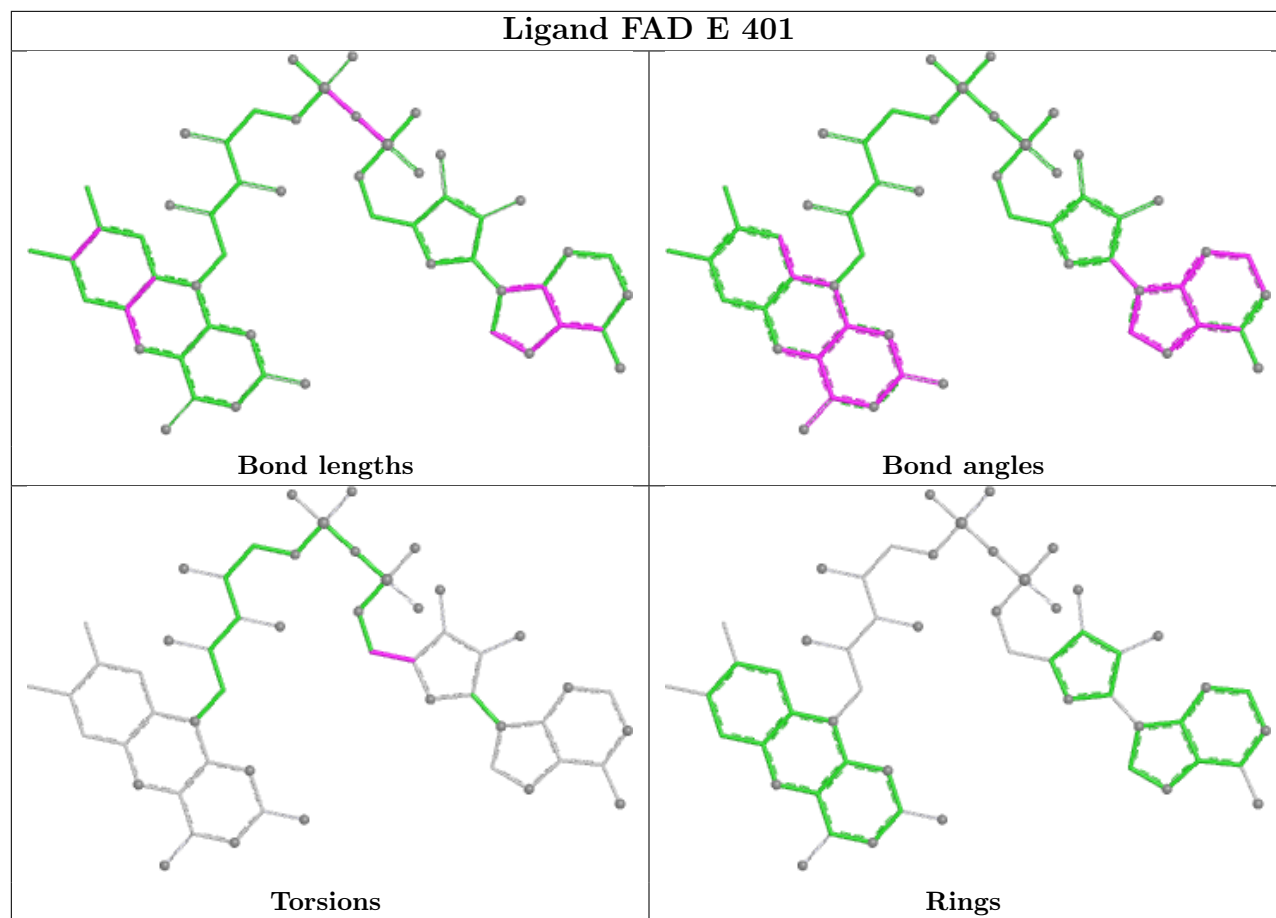
Bond angles

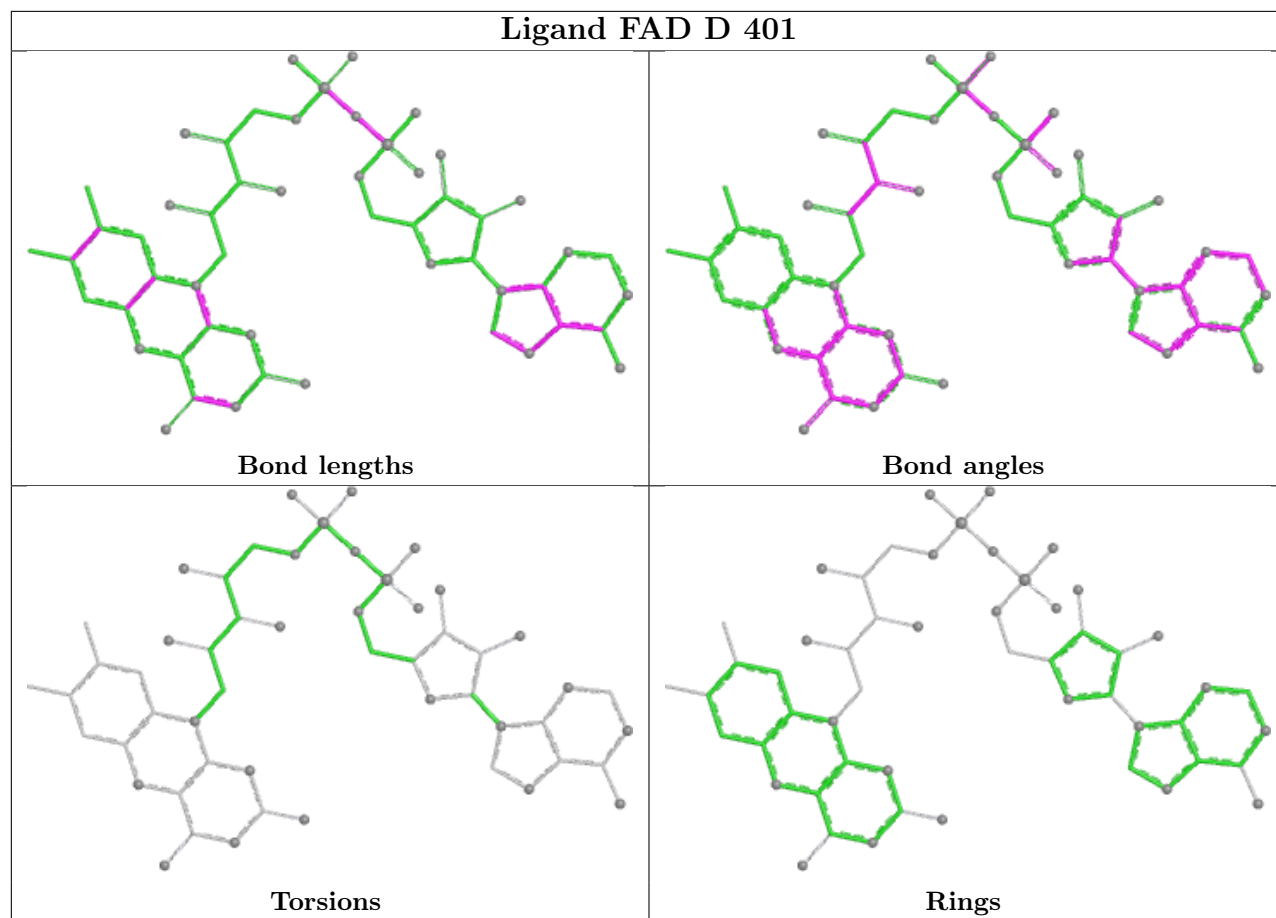


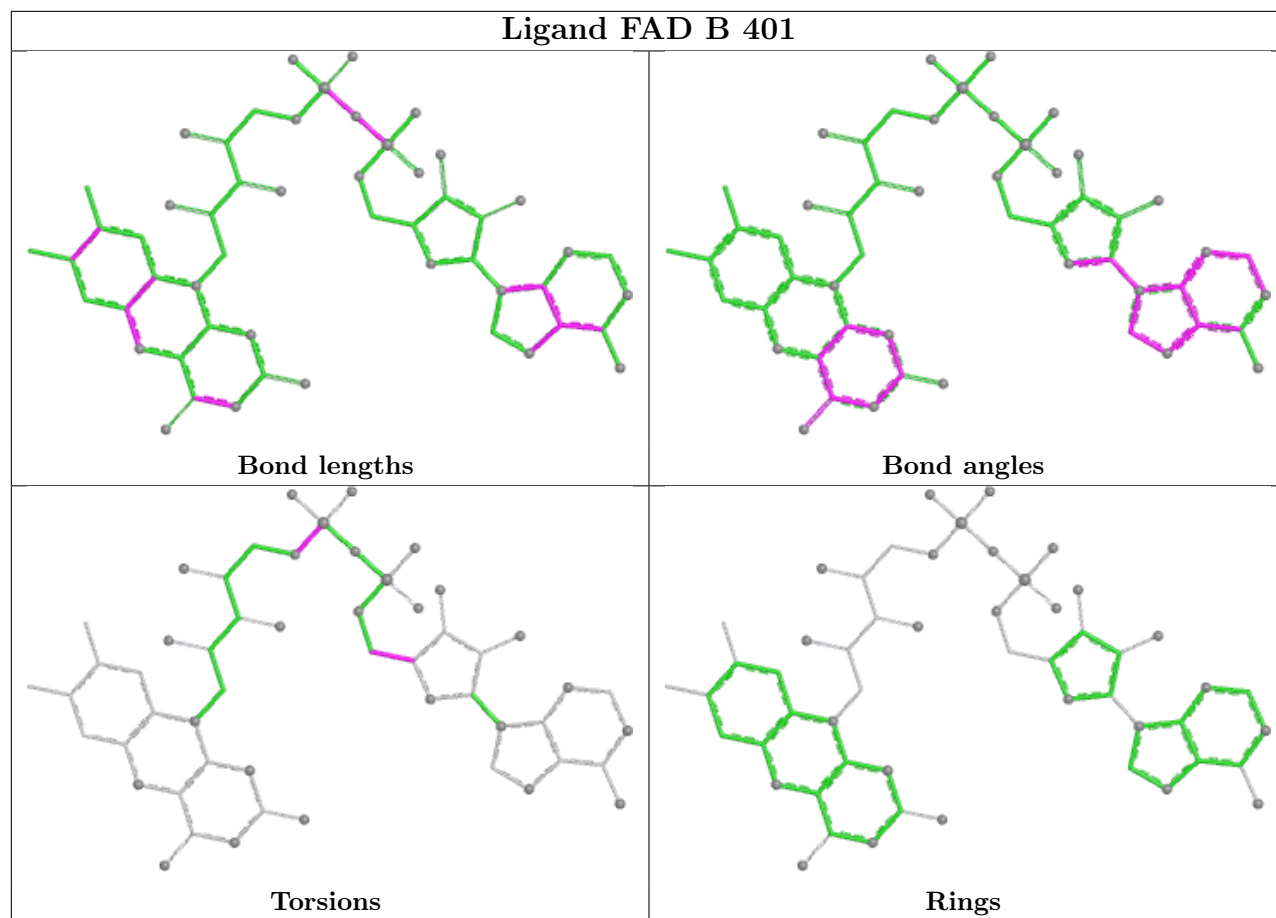
Torsions

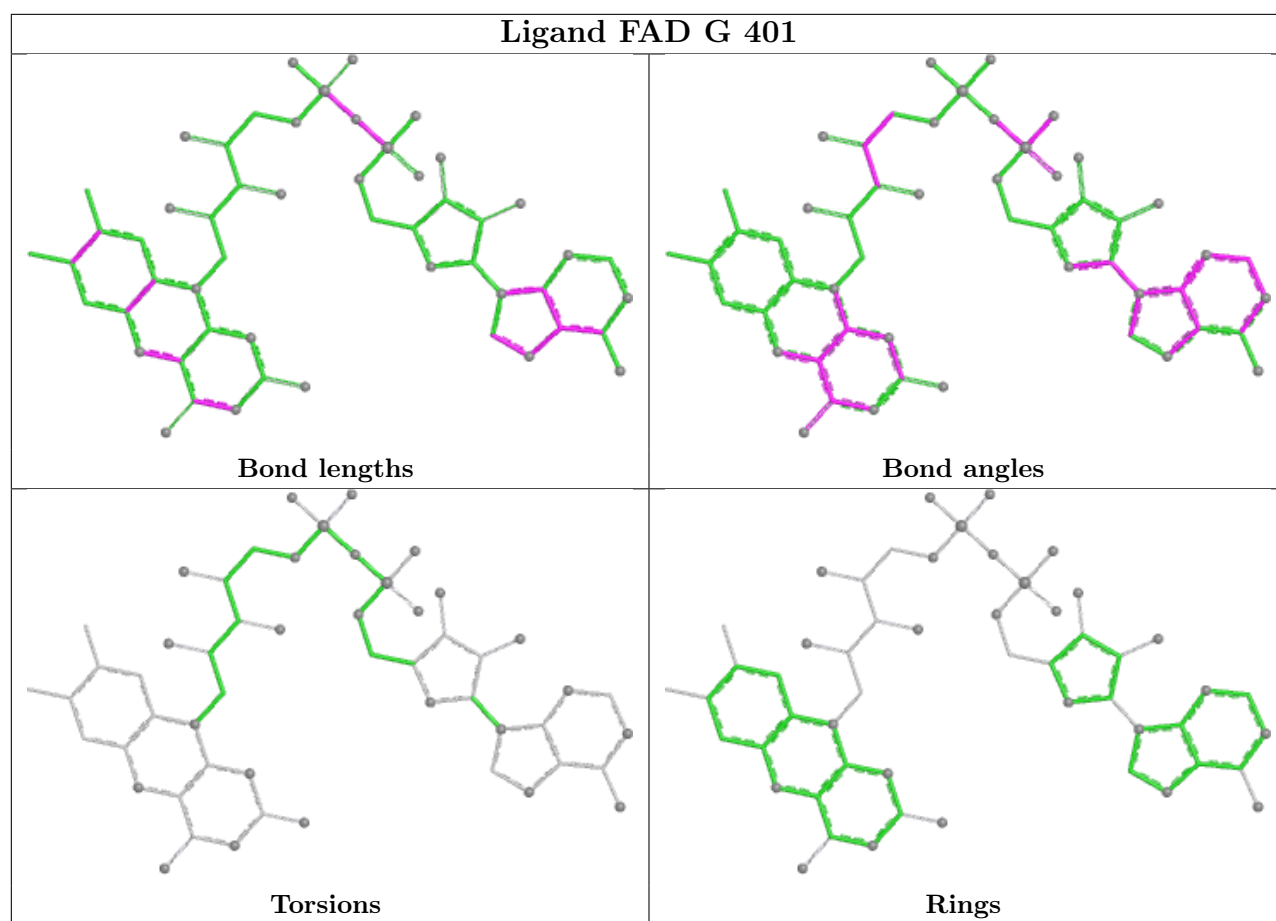


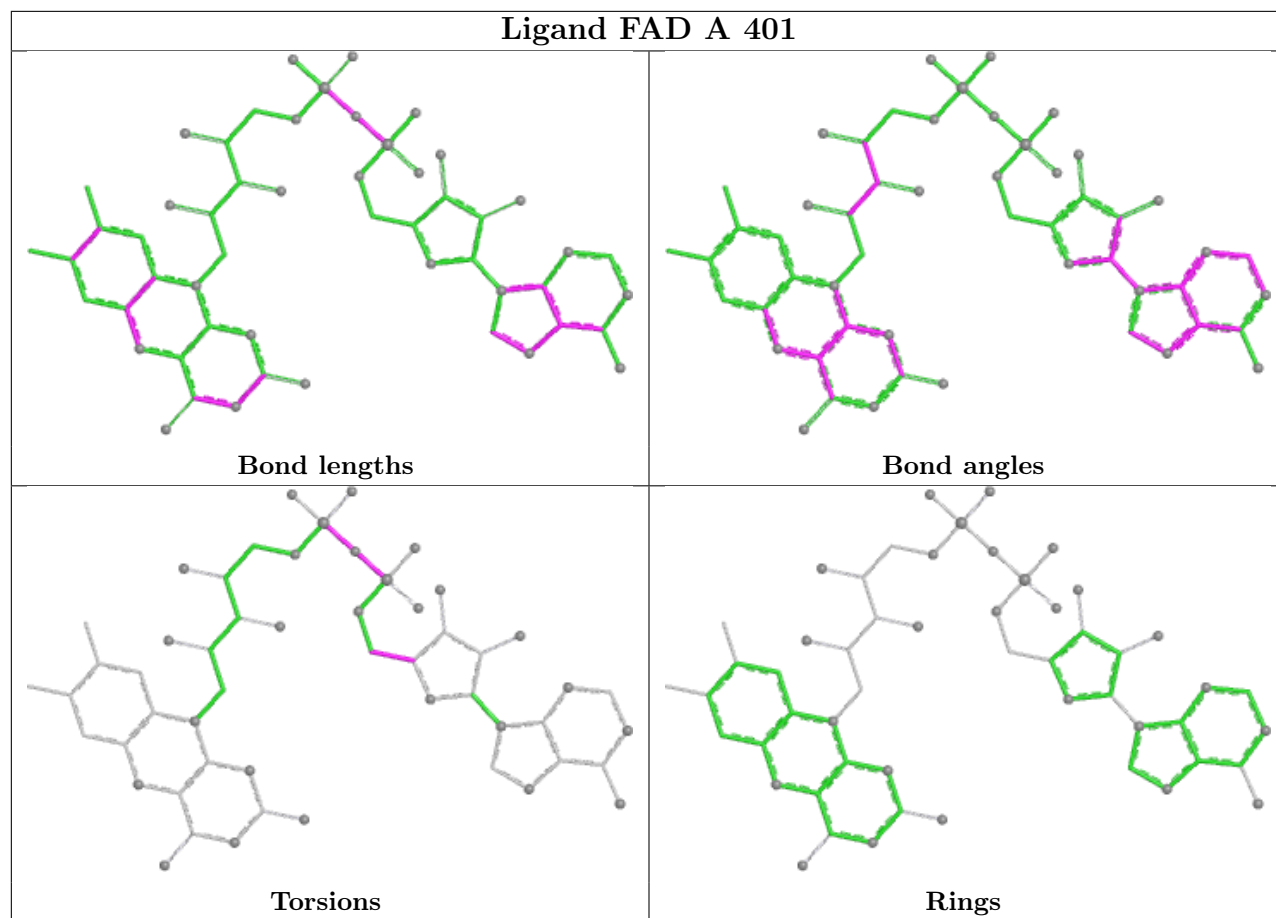
Rings

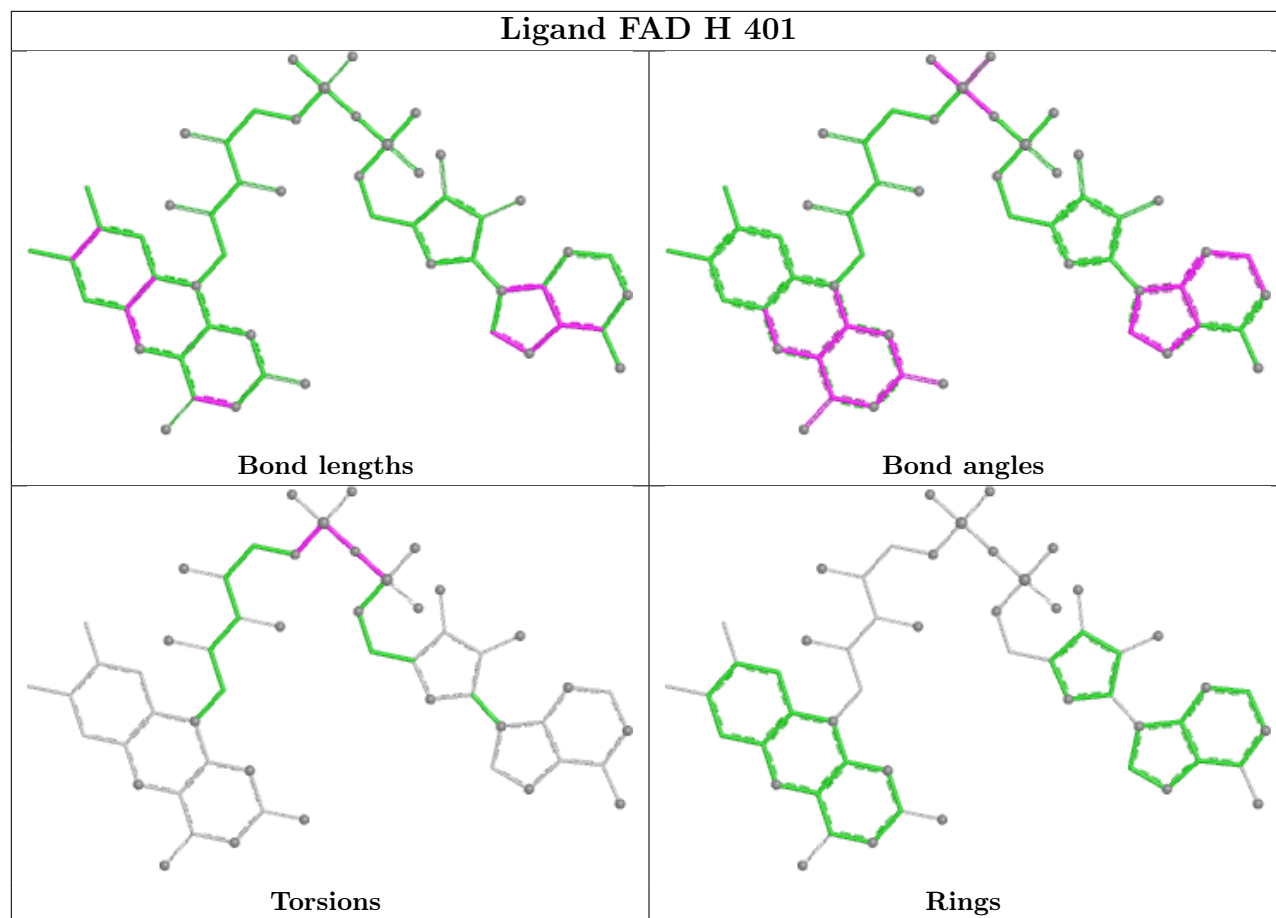












5.7 Other polymers [i](#)

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	337/347 (97%)	-0.72	0	100	100	28, 44, 91, 128	1 (0%)
1	B	339/347 (97%)	-0.67	0	100	100	26, 49, 85, 114	0
1	C	339/347 (97%)	-0.63	0	100	100	36, 53, 100, 133	1 (0%)
1	D	339/347 (97%)	-0.51	1 (0%)	90	79	35, 54, 100, 135	0
1	E	339/347 (97%)	-0.51	0	100	100	31, 65, 110, 157	2 (0%)
1	F	339/347 (97%)	-0.40	0	100	100	41, 73, 115, 140	0
1	G	338/347 (97%)	-0.46	1 (0%)	90	79	41, 67, 113, 137	1 (0%)
1	H	337/347 (97%)	-0.40	1 (0%)	90	79	46, 69, 112, 155	1 (0%)
All	All	2707/2776 (97%)	-0.54	3 (0%)	92	86	26, 60, 106, 157	6 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	219	LEU	2.5
1	D	29	PRO	2.0
1	H	29	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

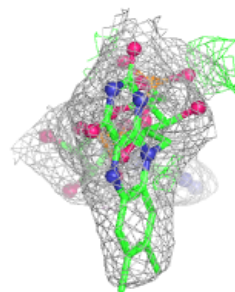
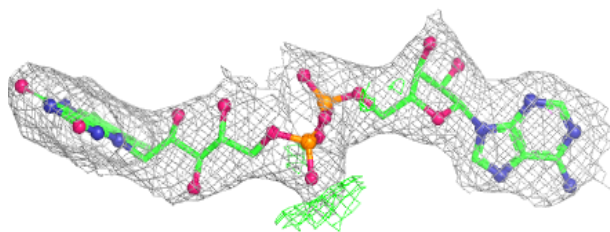
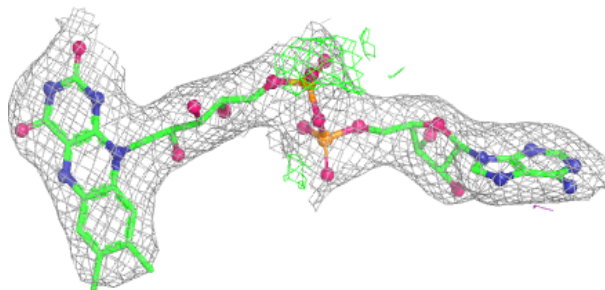
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	D	405	5/5	0.78	0.14	102,106,108,111	0
3	MPD	B	405	8/8	0.83	0.19	73,78,83,84	0
3	MPD	F	402	8/8	0.86	0.19	77,84,90,94	0
3	MPD	D	404	8/8	0.87	0.15	101,111,113,115	0
3	MPD	D	403	8/8	0.89	0.18	87,92,95,96	0
3	MPD	F	405	8/8	0.89	0.14	84,89,90,92	0
3	MPD	A	402	8/8	0.89	0.20	72,76,80,85	0
4	SO4	F	406	5/5	0.89	0.08	98,99,105,107	0
3	MPD	G	402	8/8	0.90	0.14	58,65,68,71	0
3	MPD	H	403	8/8	0.91	0.14	53,64,69,73	0
3	MPD	B	404	8/8	0.91	0.17	64,74,79,86	0
3	MPD	F	403	8/8	0.91	0.15	74,77,78,80	0
4	SO4	H	404	5/5	0.91	0.11	83,87,91,96	0
3	MPD	A	405	8/8	0.92	0.15	64,73,75,76	0
3	MPD	C	402	8/8	0.92	0.14	47,51,52,55	0
3	MPD	B	402	8/8	0.93	0.14	52,63,67,68	0
4	SO4	C	403	5/5	0.93	0.07	62,71,76,76	0
3	MPD	G	403	8/8	0.93	0.15	79,83,86,89	0
4	SO4	E	403	5/5	0.93	0.07	93,98,105,105	0
3	MPD	G	404	8/8	0.93	0.12	83,91,93,93	0
3	MPD	H	402	8/8	0.93	0.16	82,86,89,92	0
3	MPD	F	404	8/8	0.94	0.13	55,64,72,73	0
3	MPD	E	402	8/8	0.94	0.16	79,83,85,86	0
3	MPD	B	403	8/8	0.94	0.14	78,86,90,95	0
3	MPD	A	403	8/8	0.94	0.15	51,63,69,70	0
4	SO4	A	406	5/5	0.95	0.08	54,55,58,60	0
3	MPD	A	404	8/8	0.95	0.10	39,42,43,45	0
2	FAD	F	401	53/53	0.96	0.06	43,52,59,60	0
2	FAD	G	401	53/53	0.96	0.07	44,54,60,63	0
2	FAD	H	401	53/53	0.96	0.07	41,46,52,56	0
2	FAD	E	401	53/53	0.97	0.06	41,49,54,58	0
3	MPD	D	402	8/8	0.97	0.10	53,61,64,65	0
2	FAD	B	401	53/53	0.97	0.06	33,37,45,47	0
2	FAD	C	401	53/53	0.97	0.06	35,42,46,49	0
2	FAD	D	401	53/53	0.97	0.06	29,40,47,49	0
2	FAD	A	401	53/53	0.98	0.05	28,32,35,36	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.

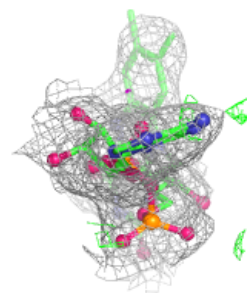
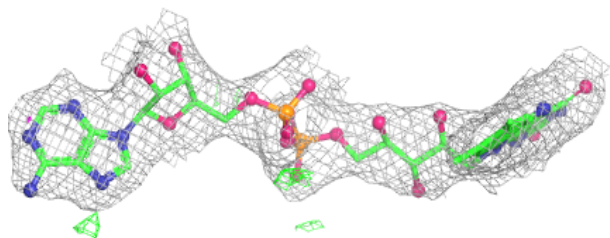
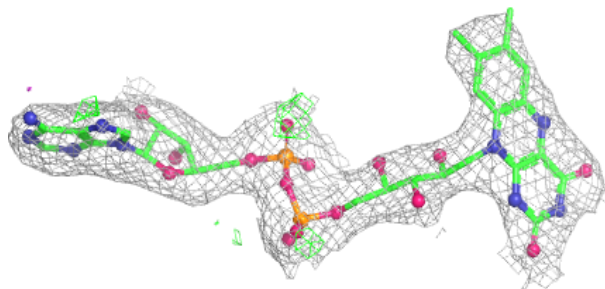
Electron density around FAD F 401:

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

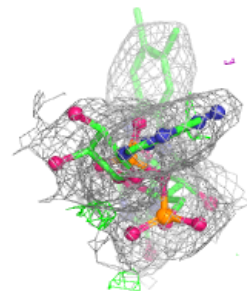
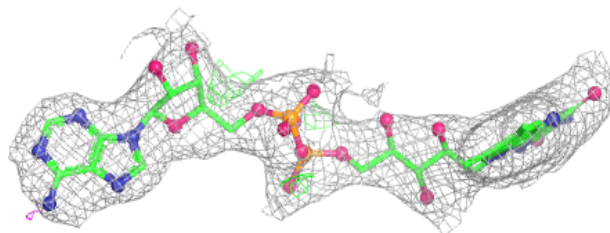
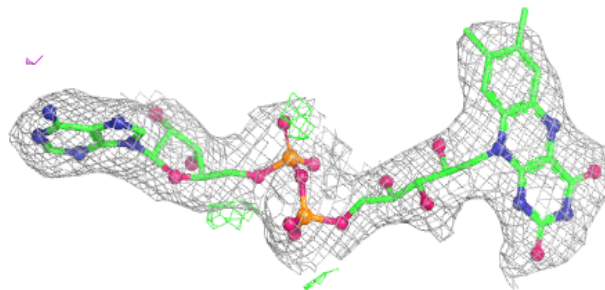


Electron density around FAD G 401:

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

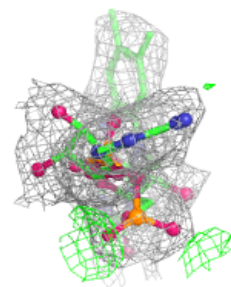
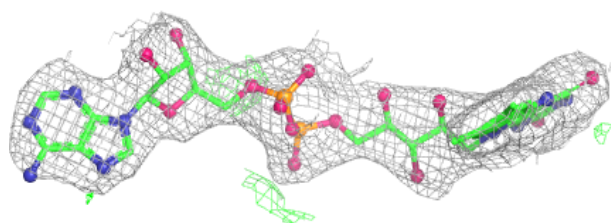
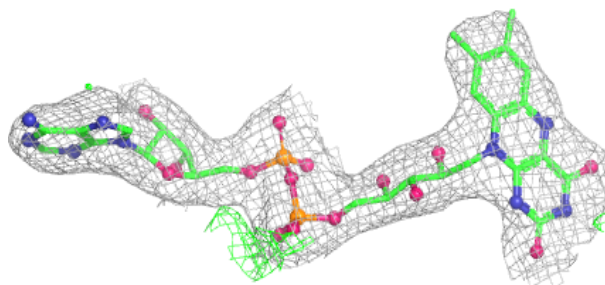
**Electron density around FAD H 401:**

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

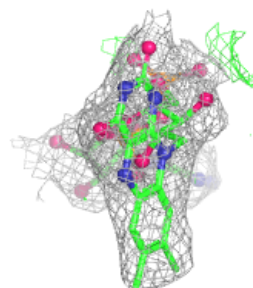
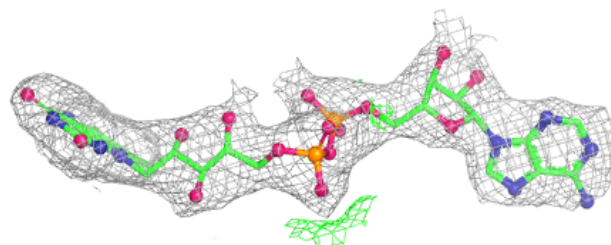
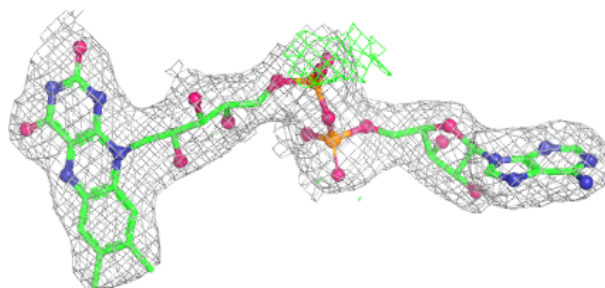


Electron density around FAD E 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

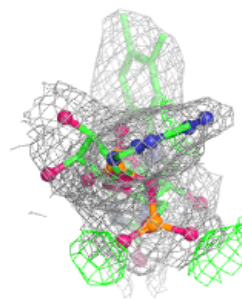
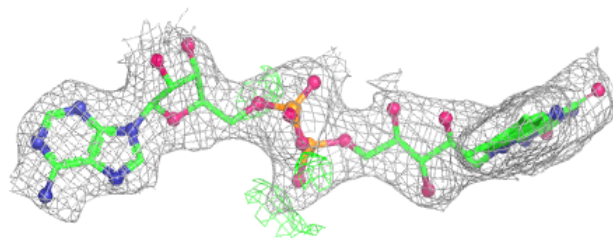
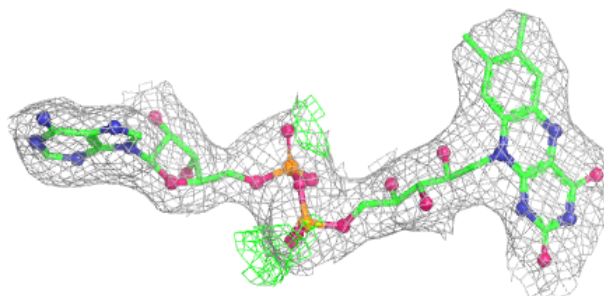
**Electron density around FAD B 401:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

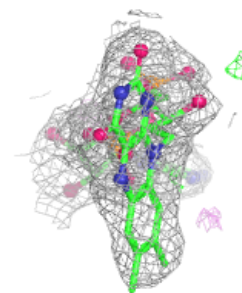
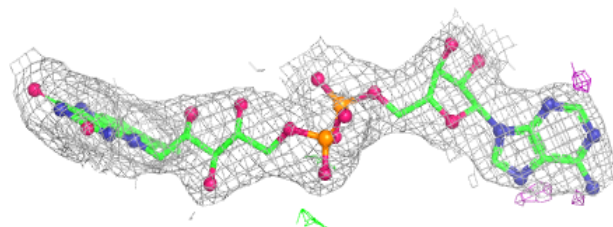
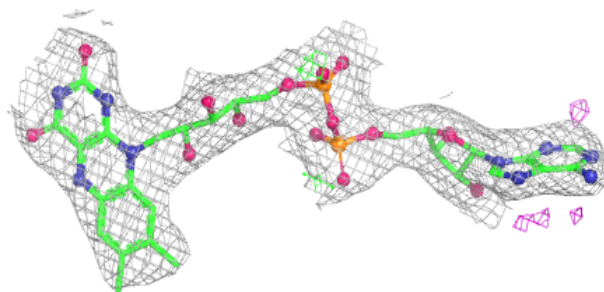


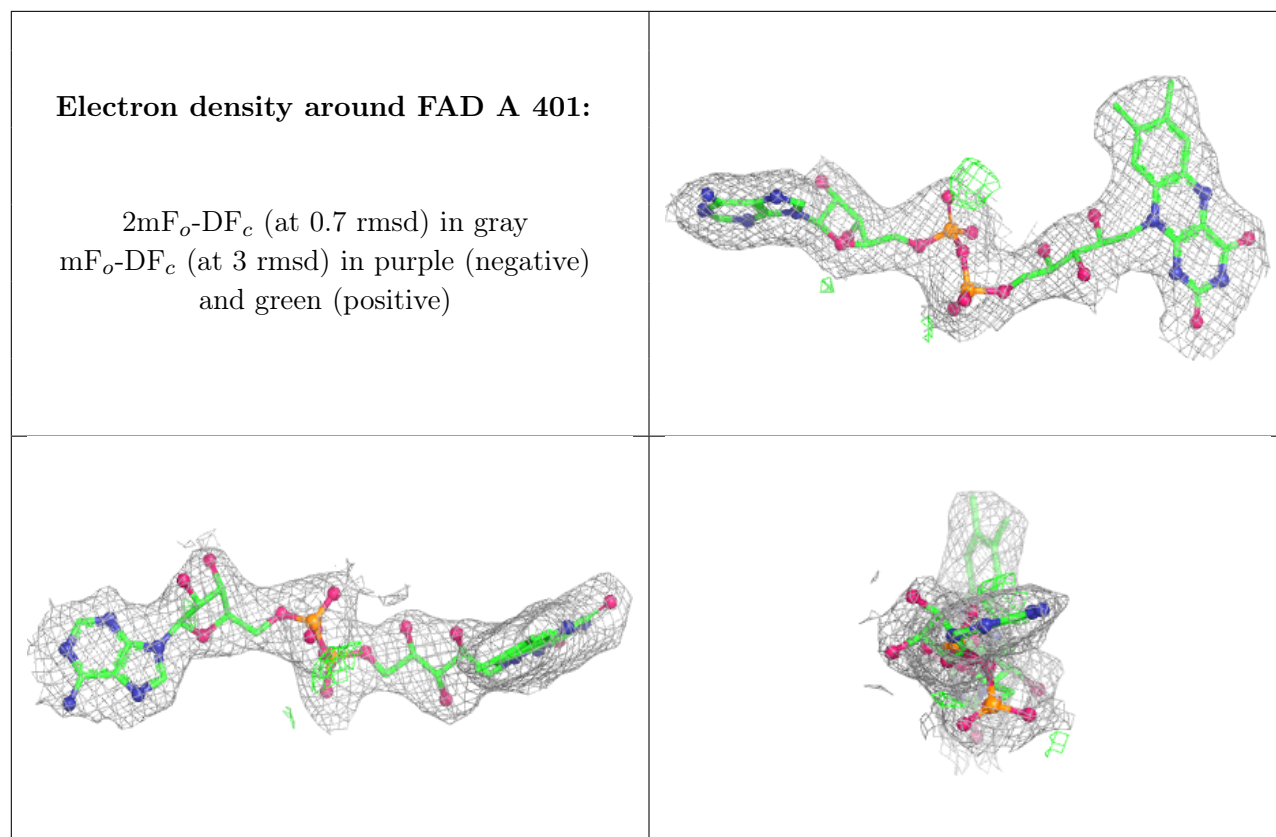
Electron density around FAD C 401:

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

**Electron density around FAD D 401:**

$2mF_o-DF_c$ (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.