Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2020 – 12:17 pm GMT

PDB ID	:	7A7B
Title	:	Bacillithiol Disulfide Reductase Bdr (YpdA) from Staphylococcus aureus
Authors	:	Hammerstad, M.; Hersleth, H.-P.
Deposited on	:	2020-08-27
Resolution	:	2.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

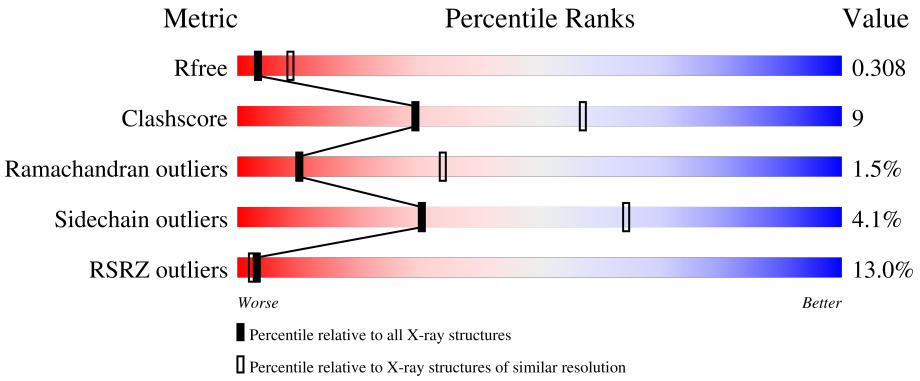
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	328	2% 78% 18%
1	B	328	4% 83% 14%
1	C	328	% 77% 20%
1	D	328	% 74% 23%
1	E	328	3% 82% 16%

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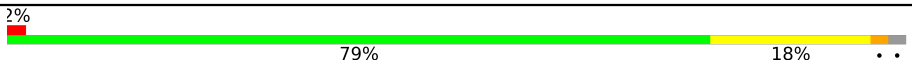
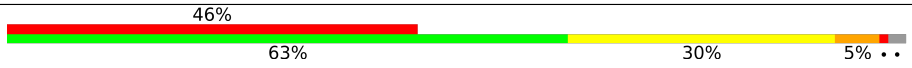
Mol	Chain	Length	Quality of chain
1	F	328	
1	G	328	
1	H	328	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	H	401	-	-	-	X
3	NAP	D	402[A]	-	-	-	X
3	NAP	D	402[B]	-	-	-	X
3	NAP	F	402	-	-	-	X

2 Entry composition (i)

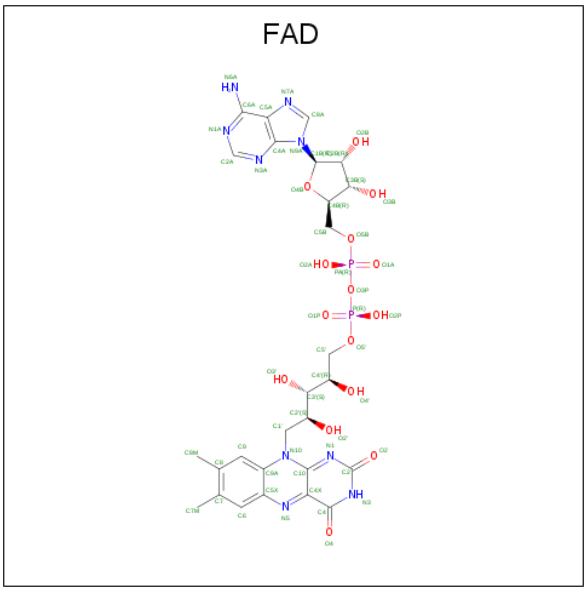
There are 4 unique types of molecules in this entry. The entry contains 20666 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 YpdA family putative bacillithiol disulfide reductase Bdr.

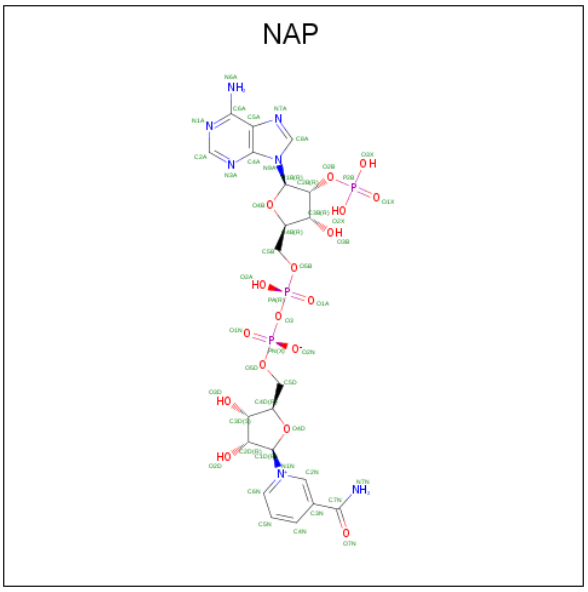
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2554	1633	420	492	9			
1	B	323	Total	C	N	O	S	0	0	0
			2554	1633	420	492	9			
1	C	323	Total	C	N	O	S	0	1	0
			2560	1637	421	493	9			
1	D	323	Total	C	N	O	S	0	1	0
			2565	1642	421	493	9			
1	E	323	Total	C	N	O	S	0	1	0
			2559	1636	421	493	9			
1	F	323	Total	C	N	O	S	0	2	0
			2565	1640	420	496	9			
1	G	265	Total	C	N	O	S	0	0	0
			2113	1350	347	408	8			
1	H	323	Total	C	N	O	S	0	0	0
			2554	1633	420	492	9			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	1
			96	42	14	34	6		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

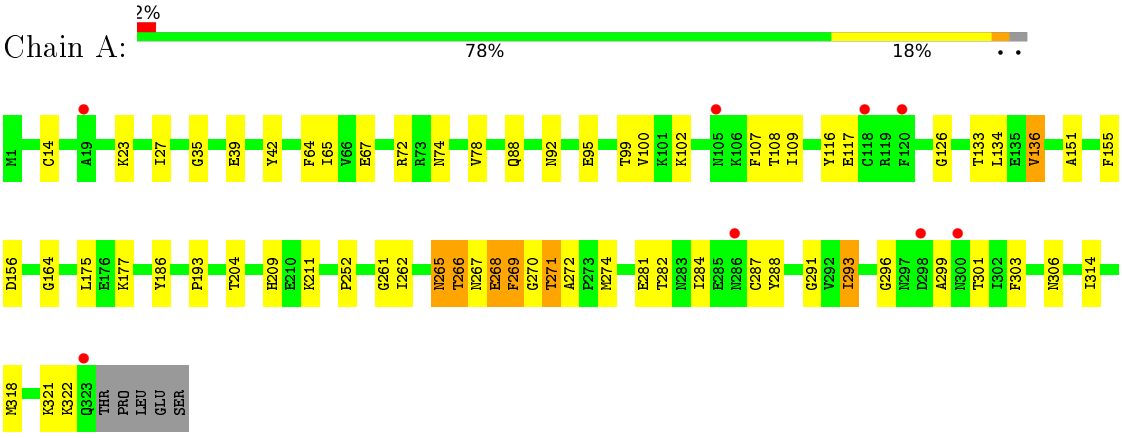
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	C	4	Total	O	0	0
			4	4		
4	D	4	Total	O	0	0
			4	4		
4	E	3	Total	O	0	0
			3	3		
4	F	4	Total	O	0	0
			4	4		
4	G	2	Total	O	0	0
			2	2		
4	H	4	Total	O	0	0
			4	4		

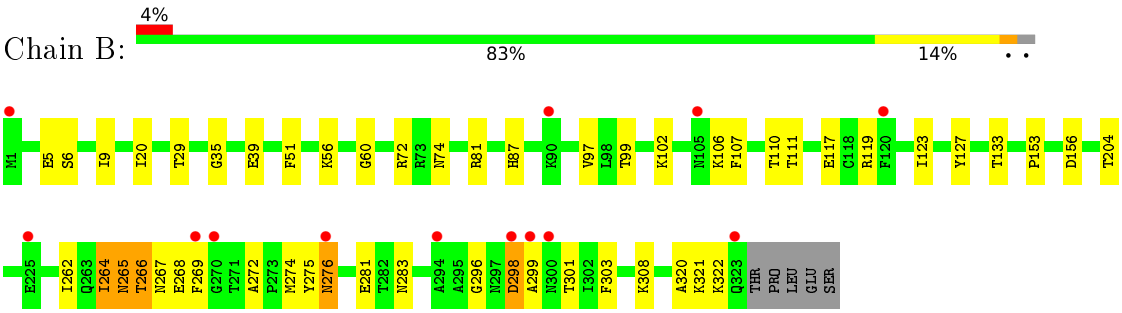
3 Residue-property plots (i)

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.

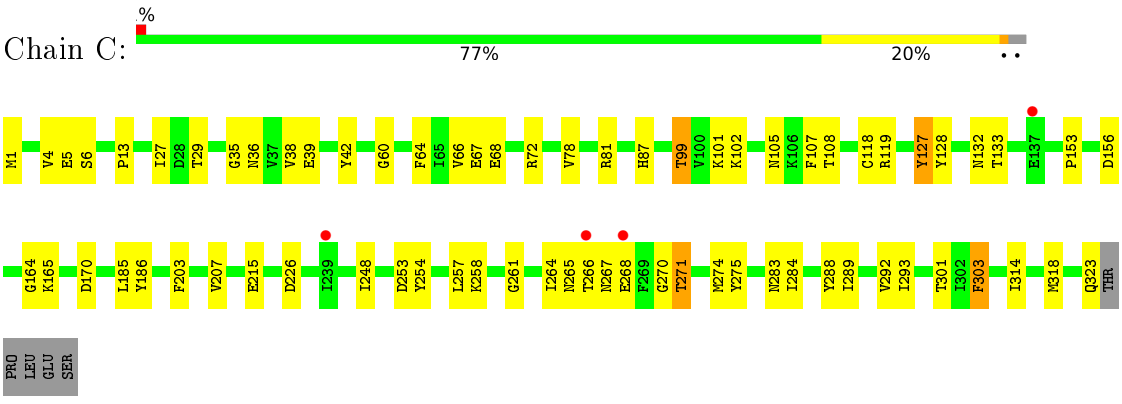
- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr



- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr

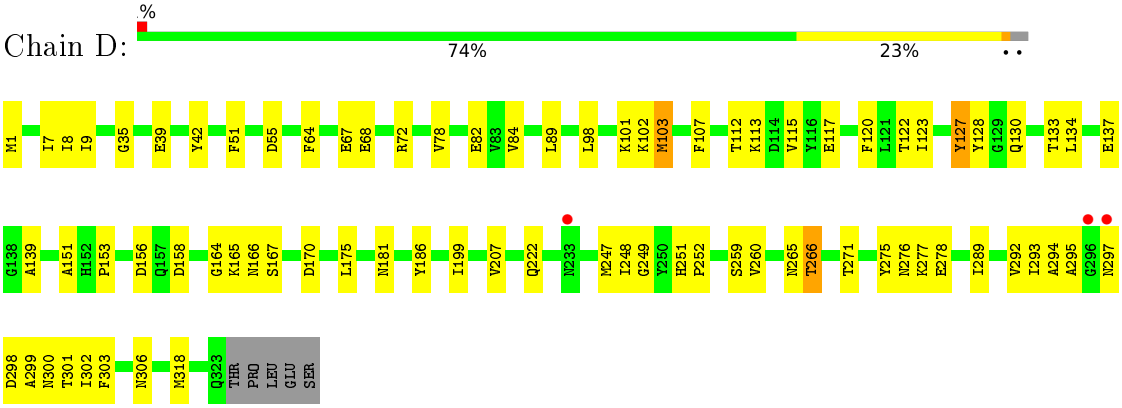


- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr



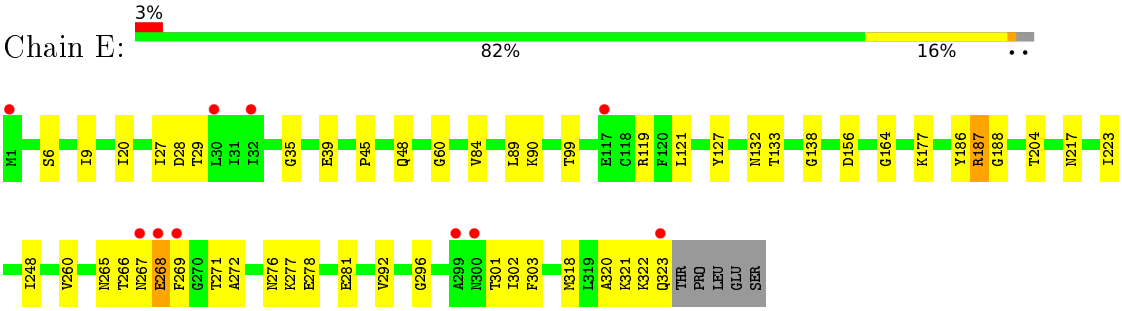
• Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr

Chain D:



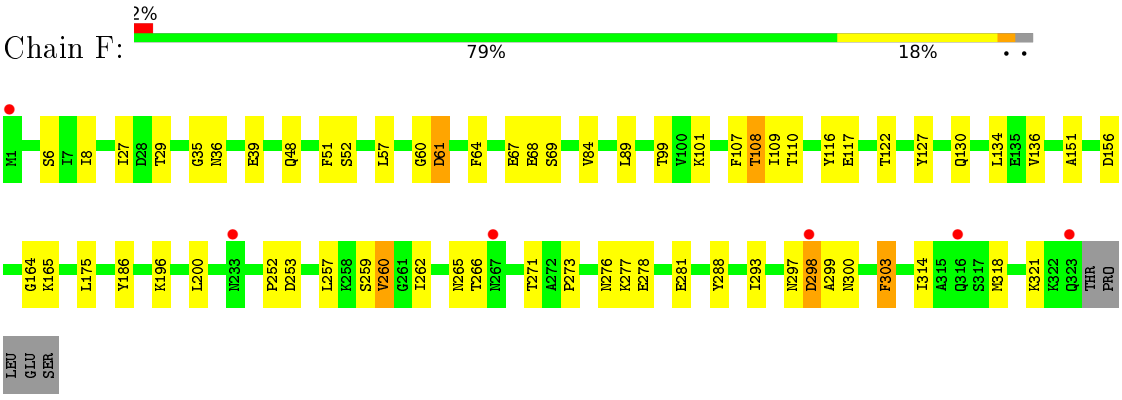
• Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr

Chain E:



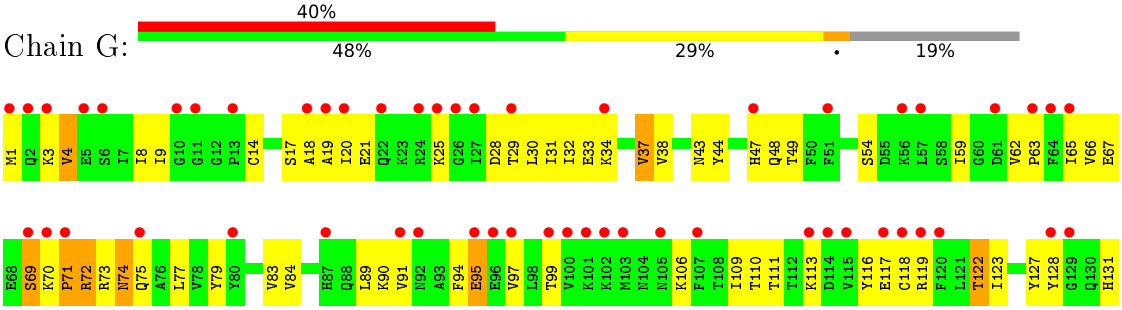
• Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr

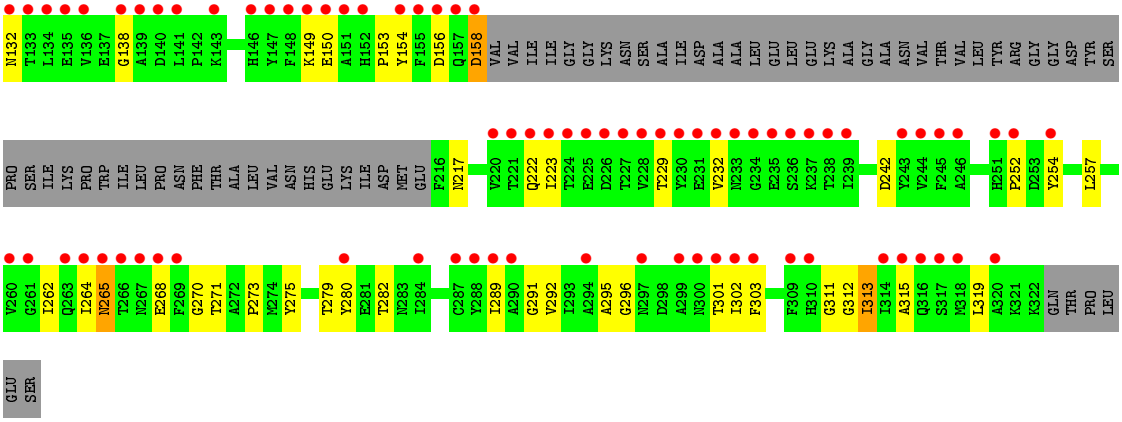
Chain F:



• Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr

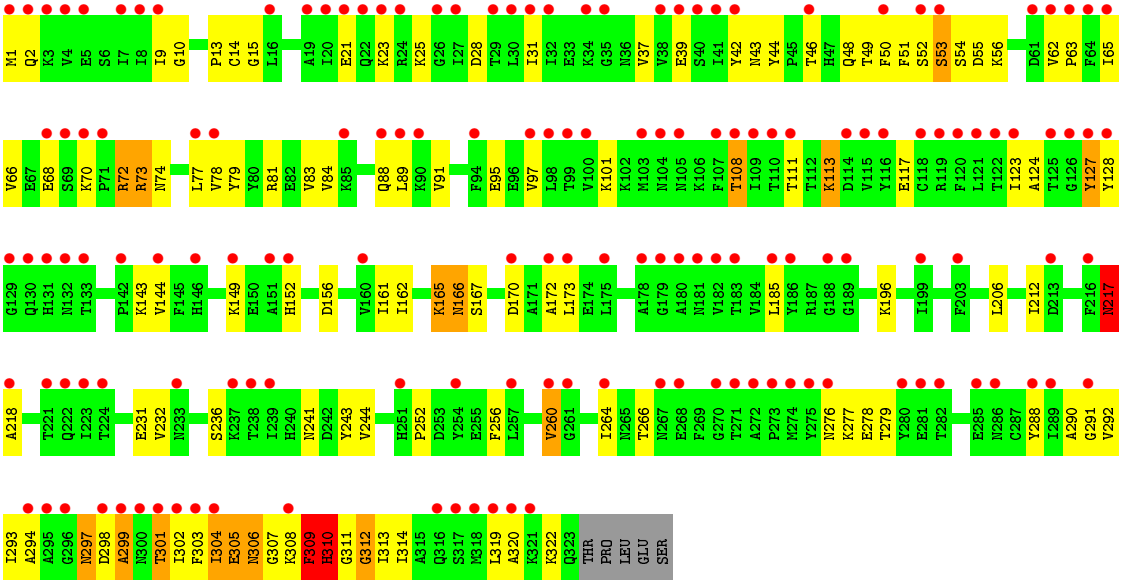
Chain G:





- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	179.31Å 179.31Å 349.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.63 – 2.90 49.63 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.63-2.90) 99.7 (49.63-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.09 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, REFMAC 5.8.0253	Depositor
R, R_{free}	0.243 , 0.308 0.243 , 0.308	Depositor DCC
R_{free} test set	3682 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	59.5	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	20666	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAP, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.49	0/2610	0.67	0/3537
1	B	0.49	0/2610	0.64	0/3537
1	C	0.54	0/2619	0.68	0/3549
1	D	0.52	0/2622	0.67	0/3553
1	E	0.53	0/2618	0.69	1/3548 (0.0%)
1	F	0.50	0/2627	0.68	1/3560 (0.0%)
1	G	0.39	0/2159	0.55	0/2921
1	H	0.44	0/2610	0.70	1/3537 (0.0%)
All	All	0.49	0/20475	0.66	3/27742 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	113	LYS	CD-CE-NZ	-5.87	98.19	111.70
1	E	187	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	F	61	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	ASN	Peptide
1	H	310	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2554	0	2506	46	0
1	B	2554	0	2506	28	0
1	C	2560	0	2514	45	0
1	D	2565	0	2514	57	0
1	E	2559	0	2512	28	0
1	F	2565	0	2516	44	0
1	G	2113	0	2058	75	0
1	H	2554	0	2506	83	0
2	A	53	0	31	3	0
2	B	53	0	31	0	0
2	C	53	0	31	3	0
2	D	53	0	31	3	0
2	E	53	0	31	0	0
2	F	53	0	31	2	0
2	G	53	0	31	5	0
2	H	53	0	31	5	0
3	C	48	0	25	4	0
3	D	96	0	50	18	0
3	F	48	0	25	6	0
4	A	5	0	0	0	0
4	C	4	0	0	1	0
4	D	4	0	0	0	0
4	E	3	0	0	0	0
4	F	4	0	0	0	0
4	G	2	0	0	1	0
4	H	4	0	0	0	0
All	All	20666	0	19980	385	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 9.

All (385) 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:H:21:GLU:HG3	1:H:310:HIS:HB3	1.52	0.90
1:H:44:TYR:HH	2:H:401:FAD:HO2'	1.09	0.85
1:D:266:THR:HG22	1:D:271:THR:HG22	1.57	0.85
1:B:60:GLY:O	1:B:87:HIS:NE2	2.11	0.83
1:B:99:THR:HB	1:B:110:THR:HB	1.59	0.83
1:G:8:ILE:HG23	1:G:122:THR:HB	1.62	0.81
1:C:105:ASN:ND2	4:C:501:HOH:O	2.16	0.77
1:H:43:ASN:HB2	1:H:128:TYR:OH	1.86	0.76
1:C:301:THR:HG23	1:E:188:GLY:HA2	1.69	0.74
1:G:257:LEU:HD22	1:G:262:ILE:HD12	1.69	0.74
1:F:134:LEU:HG	1:F:136:VAL:HG13	1.70	0.73
1:G:97:VAL:HA	1:G:111:THR:HG22	1.70	0.73
1:G:1:MET:N	4:G:501:HOH:O	2.21	0.72
1:F:51:PHE:CE2	3:F:402:NAP:H2N	2.25	0.72
1:H:311:GLY:O	1:H:313:ILE:N	2.23	0.72
1:G:8:ILE:HB	1:G:31:ILE:HG12	1.72	0.71
1:D:299:ALA:O	3:D:402[A]:NAP:O2D	2.07	0.70
1:G:37:VAL:HG23	1:G:38:VAL:HG22	1.72	0.70
1:A:269:PHE:CE2	1:A:299:ALA:HB2	2.26	0.70
1:H:62:VAL:HG21	1:H:83:VAL:HG22	1.73	0.70
1:H:73:ARG:HH11	1:H:77:LEU:HD11	1.57	0.70
1:H:292:VAL:HG13	1:H:304:ILE:HD12	1.74	0.69
1:B:272:ALA:HB2	1:B:296:GLY:HA3	1.73	0.69
1:C:265:ASN:ND2	1:C:274:MET:SD	2.66	0.68
1:D:164:GLY:H	3:D:402[A]:NAP:H4B	1.59	0.68
1:G:28:ASP:OD1	1:G:90:LYS:NZ	2.22	0.68
1:A:35:GLY:HA3	1:A:39:GLU:HG3	1.75	0.68
1:G:49:THR:HG23	1:G:72:ARG:HG2	1.75	0.68
1:F:165:LYS:HD3	3:F:402:NAP:O1A	1.94	0.67
1:E:35:GLY:HA3	1:E:39:GLU:HG3	1.76	0.67
1:H:25:LYS:HD2	1:H:319:LEU:HD22	1.76	0.67
1:C:257:LEU:HD11	1:C:293:ILE:HD11	1.77	0.67
1:C:6:SER:HB3	1:C:29:THR:HG22	1.78	0.66
1:H:301:THR:HB	1:H:302:ILE:HD12	1.77	0.66
1:B:9:ILE:HD12	1:B:123:ILE:HG13	1.78	0.66
1:G:131:HIS:ND1	1:G:132:ASN:O	2.24	0.65
1:H:51:PHE:N	2:H:401:FAD:O4	2.28	0.65
1:C:36:ASN:ND2	1:D:153:PRO:O	2.23	0.65
1:D:186:TYR:OH	3:D:402[B]:NAP:O1X	2.12	0.64
1:G:72:ARG:HB2	1:H:70:LYS:HE2	1.79	0.64
1:C:119:ARG:NH2	1:C:323:GLN:HB3	2.13	0.64
1:G:95:GLU:HG2	1:G:113:LYS:HB2	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:301:THR:HG22	1:G:302:ILE:HG12	1.79	0.63
1:B:6:SER:HB3	1:B:29:THR:HG22	1.81	0.63
1:H:1:MET:HG2	1:H:2:GLN:H	1.64	0.63
1:F:303:PHE:HB2	2:F:401:FAD:O2	1.99	0.62
1:H:73:ARG:NH1	1:H:77:LEU:HD11	2.14	0.62
1:B:102:LYS:HD3	1:B:107:PHE:CE1	2.34	0.62
1:A:272:ALA:HB2	1:A:296:GLY:HA3	1.82	0.62
1:G:47:HIS:CE1	1:H:72:ARG:HH22	2.18	0.61
1:A:265:ASN:O	1:A:265:ASN:ND2	2.28	0.61
1:H:48:GLN:NE2	1:H:170:ASP:OD2	2.34	0.61
1:G:150:GLU:OE2	1:H:73:ARG:NH2	2.34	0.61
1:A:270:GLY:HA2	1:F:271:THR:HG23	1.82	0.60
1:F:252:PRO:HB3	1:F:293:ILE:CD1	2.31	0.60
1:B:35:GLY:HA3	1:B:39:GLU:HG3	1.83	0.60
1:H:173:LEU:HD23	1:H:206:LEU:HD12	1.83	0.60
1:E:28:ASP:OD1	1:E:90:LYS:NZ	2.31	0.60
1:E:9:ILE:HD11	1:E:121:LEU:HD11	1.82	0.60
1:F:51:PHE:HE2	3:F:402:NAP:H2N	1.65	0.60
1:D:84:VAL:HG13	1:D:89:LEU:HB2	1.84	0.60
1:G:31:ILE:O	1:G:91:VAL:HA	2.00	0.60
1:H:276:ASN:O	1:H:278:GLU:N	2.35	0.60
1:B:74:ASN:ND2	1:C:67:GLU:OE1	2.31	0.60
1:H:165:LYS:O	1:H:167:SER:N	2.35	0.59
1:G:49:THR:HA	1:G:72:ARG:HA	1.83	0.59
1:F:84:VAL:HG13	1:F:89:LEU:HB2	1.85	0.59
1:G:109:ILE:HB	1:G:116:TYR:HB2	1.84	0.59
1:A:262:ILE:HD13	1:A:282:THR:HG21	1.84	0.58
1:A:27:ILE:HG21	1:A:318:MET:HE1	1.86	0.58
1:F:6:SER:HB3	1:F:29:THR:HG22	1.85	0.58
1:H:14:CYS:SG	1:H:304:ILE:HD13	2.43	0.58
1:B:264:ILE:HG22	1:B:265:ASN:H	1.69	0.58
1:H:52:SER:O	1:H:54:SER:N	2.36	0.58
1:G:262:ILE:HG21	1:G:273:PRO:HB3	1.85	0.58
1:H:231:GLU:HG2	1:H:236:SER:HA	1.86	0.57
1:H:310:HIS:HB2	1:H:312:GLY:HA3	1.85	0.57
1:A:134:LEU:HG	1:A:136:VAL:HG13	1.84	0.57
1:G:70:LYS:C	1:G:72:ARG:H	2.07	0.57
1:D:165:LYS:HD2	3:D:402[B]:NAP:H51A	1.85	0.57
1:C:292:VAL:HG13	2:C:401:FAD:H5'2	1.86	0.57
1:C:267:ASN:OD1	1:C:270:GLY:N	2.37	0.57
1:B:107:PHE:O	1:B:117:GLU:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:ARG:HB2	1:H:70:LYS:CE	2.35	0.56
1:B:72:ARG:NH2	1:C:67:GLU:OE2	2.37	0.56
1:G:254:TYR:OH	1:G:271:THR:O	2.21	0.56
1:H:72:ARG:HG3	1:H:73:ARG:H	1.70	0.56
1:E:281:GLU:OE2	1:E:321:LYS:NZ	2.38	0.56
1:A:72:ARG:NH1	1:D:67:GLU:OE2	2.38	0.56
1:F:299:ALA:O	3:F:402:NAP:O3D	2.24	0.56
1:H:56:LYS:HB3	1:H:306:ASN:HB2	1.88	0.56
1:H:78:VAL:HG22	1:H:81:ARG:HH22	1.70	0.56
1:C:127:TYR:HE1	1:C:128:TYR:CZ	2.24	0.55
1:E:164:GLY:HA3	1:E:186:TYR:CD1	2.42	0.55
1:C:267:ASN:OD1	1:C:271:THR:N	2.38	0.55
1:H:54:SER:OG	1:H:54:SER:O	2.21	0.55
1:G:9:ILE:HD13	1:G:97:VAL:HG11	1.87	0.55
1:H:252:PRO:HB3	1:H:293:ILE:HD12	1.89	0.55
1:E:29:THR:O	1:E:90:LYS:HD2	2.06	0.55
1:G:75:GLN:O	1:G:79:TYR:N	2.36	0.55
1:E:27:ILE:HD13	1:E:318:MET:HE2	1.88	0.55
1:D:98:LEU:HD11	1:D:112:THR:HG22	1.88	0.55
1:H:101:LYS:HB2	1:H:108:THR:HG23	1.89	0.55
1:H:65:ILE:HG12	1:H:66:VAL:H	1.71	0.55
1:F:68[A]:GLU:HG3	1:F:69:SER:H	1.71	0.55
1:G:25:LYS:HG3	1:G:315:ALA:HB1	1.89	0.55
1:G:74:ASN:HA	1:G:77:LEU:HB3	1.89	0.55
1:G:70:LYS:HB2	1:G:72:ARG:HG3	1.89	0.54
1:E:119:ARG:HH22	1:E:323:GLN:HB3	1.69	0.54
1:C:35:GLY:HA3	1:C:39:GLU:HG3	1.89	0.54
1:F:99:THR:OG1	1:F:110:THR:HB	2.06	0.54
1:G:8:ILE:N	1:G:30:LEU:O	2.37	0.54
1:G:18:ALA:HA	1:G:311:GLY:HA3	1.90	0.54
1:D:165:LYS:HD2	3:D:402[B]:NAP:H3B	1.90	0.54
1:E:132:ASN:ND2	1:E:248:ILE:O	2.31	0.54
1:F:281:GLU:OE2	1:F:321:LYS:NZ	2.41	0.54
1:D:170:ASP:OD2	3:D:402[B]:NAP:H4N	2.08	0.53
1:H:23:LYS:NZ	1:H:88:GLN:O	2.41	0.53
1:G:54:SER:OG	1:G:71:PRO:HB3	2.09	0.53
1:G:109:ILE:O	1:G:116:TYR:N	2.32	0.53
1:H:143:LYS:NZ	1:H:241:ASN:O	2.40	0.53
1:A:288:TYR:CD2	1:A:314:ILE:HG23	2.43	0.53
1:D:35:GLY:HA3	1:D:39:GLU:HG3	1.91	0.53
1:B:56:LYS:O	1:B:308:LYS:NZ	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:402:NAP:H6N	3:C:402:NAP:O5D	2.08	0.53
1:B:102:LYS:HD2	1:B:106:LYS:O	2.08	0.53
1:A:261:GLY:C	1:A:284:ILE:HD11	2.29	0.53
1:F:35:GLY:HA3	1:F:39:GLU:HG3	1.90	0.53
1:H:46:THR:O	1:H:72:ARG:HB2	2.09	0.52
1:D:248:ILE:HA	3:D:402[B]:NAP:O4B	2.09	0.52
1:G:44:TYR:HB2	1:G:73:ARG:HD3	1.90	0.52
1:H:310:HIS:HB2	1:H:312:GLY:N	2.25	0.52
1:C:170:ASP:OD2	3:C:402:NAP:H4N	2.09	0.52
1:F:107:PHE:O	1:F:117:GLU:HA	2.09	0.52
1:G:70:LYS:HD2	1:G:72:ARG:NH2	2.25	0.52
1:B:20:ILE:HD13	1:B:60:GLY:HA3	1.92	0.52
1:C:303:PHE:HB2	2:C:401:FAD:O2	2.10	0.52
1:F:276:ASN:O	1:F:278:GLU:N	2.43	0.52
1:H:9:ILE:HD12	1:H:123:ILE:HG12	1.91	0.52
1:A:65:ILE:HG12	1:D:82:GLU:HG3	1.92	0.51
1:H:310:HIS:HB2	1:H:312:GLY:CA	2.41	0.51
1:D:101:LYS:NZ	1:D:259:SER:O	2.43	0.51
1:F:257:LEU:HD13	1:F:273:PRO:HG3	1.93	0.51
1:C:153:PRO:HD3	1:D:42:TYR:CE1	2.45	0.51
1:D:8:ILE:HG12	1:D:122:THR:HB	1.93	0.51
1:E:6:SER:HB3	1:E:29:THR:HG22	1.92	0.51
1:G:106:LYS:NZ	1:G:119:ARG:HG2	2.25	0.51
1:F:252:PRO:HB3	1:F:293:ILE:HD11	1.93	0.51
1:F:288:TYR:CD2	1:F:314:ILE:HG23	2.46	0.51
1:G:33:GLU:OE2	2:G:401:FAD:O3B	2.28	0.51
1:C:266:THR:HA	1:C:271:THR:HG22	1.93	0.50
1:G:295:ALA:HB1	1:G:301:THR:HB	1.93	0.50
1:D:166:ASN:HD22	3:D:402[A]:NAP:H3D	1.76	0.50
1:A:14:CYS:SG	1:A:291:GLY:HA2	2.52	0.50
1:D:127:TYR:HE1	1:D:128:TYR:CZ	2.30	0.50
1:D:51[A]:PHE:CE1	1:D:199:ILE:HD11	2.47	0.50
1:F:260:VAL:HG22	1:F:262:ILE:HG13	1.94	0.50
1:H:291:GLY:HA2	1:H:304:ILE:HD11	1.93	0.50
1:D:130:GLN:HB2	1:D:251:HIS:O	2.12	0.50
1:H:21:GLU:HG3	1:H:310:HIS:CB	2.35	0.50
1:G:106:LYS:HZ3	1:G:119:ARG:HG2	1.77	0.50
1:H:297:ASN:O	1:H:299:ALA:N	2.44	0.50
1:G:9:ILE:HG23	1:G:97:VAL:HG21	1.94	0.49
1:F:164:GLY:HA3	1:F:186:TYR:CD1	2.47	0.49
1:A:266:THR:HB	1:A:271:THR:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:HA	1:D:78:VAL:HG21	1.94	0.49
1:C:275:TYR:CD1	1:C:289:ILE:HD11	2.47	0.49
1:D:134:LEU:HB3	1:D:139:ALA:HB1	1.95	0.49
1:F:48:GLN:HG2	2:F:401:FAD:HM72	1.95	0.49
1:F:252:PRO:HB3	1:F:293:ILE:HD12	1.94	0.49
1:G:70:LYS:O	1:G:72:ARG:N	2.45	0.49
1:G:84:VAL:HG22	1:G:89:LEU:HD12	1.93	0.49
1:F:101:LYS:NZ	1:F:259:SER:O	2.42	0.49
1:A:269:PHE:H	1:F:297:ASN:ND2	2.11	0.49
1:A:303:PHE:HB3	2:A:401:FAD:O2	2.13	0.49
1:G:25:LYS:HB3	1:G:319:LEU:HD22	1.94	0.49
1:D:158:ASP:OD1	1:D:181:ASN:ND2	2.40	0.49
1:D:295:ALA:HB2	1:D:302:ILE:HG13	1.95	0.49
1:A:252:PRO:HB3	1:A:293:ILE:CD1	2.43	0.49
1:A:95:GLU:OE2	1:A:116:TYR:OH	2.18	0.49
1:G:14:CYS:SG	1:G:291:GLY:HA2	2.53	0.49
1:C:42:TYR:CE1	1:D:153:PRO:HD3	2.48	0.48
1:D:107:PHE:O	1:D:117:GLU:HA	2.13	0.48
1:D:68:GLU:OE1	1:D:72:ARG:NH2	2.27	0.48
1:G:127:TYR:HB3	1:G:252:PRO:HG3	1.94	0.48
1:A:301:THR:O	1:A:306:ASN:ND2	2.46	0.48
1:H:95:GLU:HB2	1:H:113:LYS:NZ	2.27	0.48
1:H:124:ALA:HB2	1:H:290:ALA:HB3	1.95	0.48
1:C:27:ILE:HD13	1:C:318:MET:HE2	1.94	0.48
1:E:84:VAL:HG13	1:E:89:LEU:HB2	1.95	0.48
1:D:275:TYR:CD1	1:D:289:ILE:HD11	2.48	0.48
1:E:132:ASN:HB2	1:E:248:ILE:HG13	1.95	0.48
1:F:51:PHE:CD2	3:F:402:NAP:H2N	2.49	0.48
1:E:177:LYS:HE2	1:F:67:GLU:O	2.13	0.48
1:F:52:SER:HB2	1:F:57:LEU:HD21	1.96	0.48
1:A:42:TYR:CE1	1:B:153:PRO:HD3	2.49	0.48
1:C:226:ASP:N	1:C:226:ASP:OD1	2.47	0.48
1:H:218:ALA:HB2	1:H:232:VAL:HG22	1.95	0.48
1:F:165:LYS:HG3	3:F:402:NAP:O3B	2.14	0.48
1:A:268:GLU:O	1:A:269:PHE:HB2	2.14	0.48
1:A:261:GLY:CA	1:A:284:ILE:HD11	2.43	0.48
1:D:167:SER:H	3:D:402[A]:NAP:H51N	1.78	0.48
1:B:51:PHE:HZ	1:B:303:PHE:CD1	2.31	0.48
1:C:68:GLU:CD	1:C:72:ARG:HH22	2.17	0.48
1:A:193:PRO:HG3	1:F:300:ASN:HD22	1.79	0.48
1:G:69:SER:OG	1:G:70:LYS:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PHE:CD1	1:B:81:ARG:HD2	2.49	0.47
1:D:249:GLY:HA3	3:D:402[A]:NAP:O2A	2.14	0.47
1:G:275:TYR:CE2	1:G:289:ILE:HD11	2.48	0.47
1:G:4:VAL:HG21	1:G:30:LEU:HD22	1.96	0.47
1:H:218:ALA:CB	1:H:232:VAL:HG22	2.43	0.47
1:G:17:SER:HA	1:G:20:ILE:HD12	1.97	0.47
1:A:252:PRO:HB3	1:A:293:ILE:HD11	1.95	0.47
1:F:68[A]:GLU:HG3	1:F:69:SER:N	2.28	0.47
1:C:132:ASN:HB2	1:C:248:ILE:HG13	1.96	0.47
1:D:9:ILE:HD12	1:D:123:ILE:HG12	1.97	0.47
1:H:309:PHE:HB3	1:H:310:HIS:H	1.32	0.47
1:H:320:ALA:O	1:H:322:LYS:HG3	2.15	0.47
1:A:164:GLY:HA3	1:A:186:TYR:CD1	2.49	0.47
1:E:267:ASN:CG	1:E:268:GLU:H	2.18	0.47
1:G:99:THR:HB	1:G:110:THR:HB	1.97	0.47
1:D:1:MET:HB2	1:D:115:VAL:O	2.14	0.47
1:H:56:LYS:CA	1:H:306:ASN:HB2	2.44	0.47
1:A:262:ILE:HD11	1:A:287:CYS:SG	2.55	0.47
1:D:102:LYS:HD2	1:D:107:PHE:CZ	2.50	0.47
1:B:268:GLU:HB3	1:B:269:PHE:H	1.48	0.46
1:G:43:ASN:HB2	1:G:128:TYR:HE2	1.80	0.46
1:H:49:THR:O	1:H:49:THR:HG22	2.15	0.46
1:A:126:GLY:HA3	2:A:401:FAD:O2A	2.16	0.46
1:C:203:PHE:O	1:C:207:VAL:HG23	2.16	0.46
1:G:65:ILE:HD12	1:G:65:ILE:HA	1.63	0.46
2:G:401:FAD:O4'	2:G:401:FAD:O2'	2.30	0.46
1:C:254:TYR:CD1	1:C:264:ILE:HD11	2.50	0.46
1:D:165:LYS:HD2	3:D:402[A]:NAP:O5B	2.14	0.46
1:H:256:PHE:O	1:H:260:VAL:HG13	2.15	0.46
1:C:268:GLU:HG3	1:E:132:ASN:HD21	1.81	0.46
1:A:23:LYS:NZ	1:A:88:GLN:O	2.50	0.45
1:C:60:GLY:O	1:C:87:HIS:NE2	2.29	0.45
1:H:1:MET:SD	1:H:117:GLU:HB2	2.57	0.45
1:D:128:TYR:OH	2:D:401:FAD:H9	2.16	0.45
1:C:4:VAL:O	1:C:118:CYS:HA	2.15	0.45
1:D:165:LYS:HB3	3:D:402[A]:NAP:O3D	2.17	0.45
1:C:99:THR:HG23	1:C:101:LYS:HE2	1.97	0.45
1:H:31:ILE:HB	1:H:91:VAL:HG22	1.99	0.45
1:D:165:LYS:HG3	3:D:402[B]:NAP:H3B	1.98	0.45
1:G:313:ILE:HD13	1:G:313:ILE:HA	1.79	0.45
1:G:59:ILE:HG13	1:G:83:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ILE:HA	1:B:283:ASN:HD21	1.81	0.45
1:D:297:ASN:O	1:D:299:ALA:N	2.50	0.45
1:G:21:GLU:HG3	1:G:312:GLY:HA2	1.99	0.45
1:A:266:THR:HA	1:A:271:THR:HA	1.98	0.45
1:B:298:ASP:OD1	1:B:299:ALA:N	2.50	0.45
1:E:322:LYS:HE3	1:E:322:LYS:HB2	1.46	0.45
1:G:262:ILE:HD13	1:G:282:THR:HG21	1.99	0.45
1:H:14:CYS:SG	1:H:291:GLY:HA2	2.57	0.45
1:H:39:GLU:O	1:H:42:TYR:HB3	2.17	0.45
1:C:13:PRO:HD3	1:C:38:VAL:HG12	2.00	0.45
1:C:164:GLY:HA3	1:C:186:TYR:CE1	2.53	0.44
1:C:253:ASP:O	1:C:257:LEU:HD12	2.17	0.44
1:C:165:LYS:HD3	3:C:402:NAP:O1A	2.17	0.44
1:D:151:ALA:HB1	1:D:175:LEU:HA	1.99	0.44
1:F:271:THR:N	1:F:297:ASN:OD1	2.48	0.44
1:G:222:GLN:HB3	1:G:229:THR:HB	1.99	0.44
1:G:153:PRO:HG2	1:G:154:TYR:CE2	2.52	0.44
1:F:196:LYS:HA	1:F:196:LYS:HD3	1.81	0.44
1:A:269:PHE:H	1:F:297:ASN:HD21	1.65	0.44
1:C:288:TYR:CD2	1:C:314:ILE:HG23	2.52	0.44
1:F:27:ILE:HG21	1:F:318:MET:CE	2.48	0.44
1:A:14:CYS:HB2	2:A:401:FAD:O1P	2.18	0.44
2:D:401:FAD:HM73	3:D:402[B]:NAP:C4N	2.48	0.44
1:H:72:ARG:HE	1:H:73:ARG:CZ	2.31	0.44
1:D:103:MET:HE2	1:D:103:MET:HB3	1.82	0.44
1:D:275:TYR:CZ	1:D:294:ALA:HB1	2.53	0.44
1:D:276:ASN:O	1:D:278:GLU:N	2.51	0.44
1:H:144:VAL:HG22	1:H:244:VAL:HB	2.00	0.44
1:H:1:MET:HG2	1:H:2:GLN:N	2.31	0.44
1:E:20:ILE:HD13	1:E:60:GLY:HA3	2.00	0.44
1:B:5:GLU:HA	1:B:119:ARG:HD2	2.00	0.43
1:B:272:ALA:HB2	1:B:296:GLY:CA	2.47	0.43
1:E:272:ALA:HB2	1:E:296:GLY:HA3	2.00	0.43
1:F:27:ILE:HD13	1:F:318:MET:CE	2.49	0.43
1:D:55:ASP:OD1	1:D:55:ASP:N	2.50	0.43
1:H:166:ASN:HD21	1:H:196:LYS:HG2	1.82	0.43
1:D:252:PRO:HB3	1:D:293:ILE:CD1	2.48	0.43
1:G:48:GLN:HG2	2:G:401:FAD:HM72	2.01	0.43
1:H:291:GLY:C	1:H:304:ILE:HD11	2.38	0.43
1:H:161:ILE:HD12	1:H:172:ALA:HB2	2.01	0.43
1:H:162:ILE:HA	1:H:185:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:VAL:HG22	1:H:111:THR:HG22	2.00	0.43
1:E:268:GLU:HB3	1:E:269:PHE:H	1.56	0.43
1:F:130:GLN:NE2	1:F:253:ASP:HB2	2.34	0.43
2:H:401:FAD:H1'1	2:H:401:FAD:H9	1.87	0.43
1:G:150:GLU:OE1	1:H:72:ARG:NH1	2.52	0.43
1:H:124:ALA:HA	1:H:290:ALA:O	2.18	0.43
1:H:43:ASN:HB2	1:H:128:TYR:HH	1.81	0.43
1:B:97:VAL:HG22	1:B:111:THR:HG22	2.01	0.43
1:B:275:TYR:HA	1:B:281:GLU:O	2.18	0.43
1:C:165:LYS:HD2	3:C:402:NAP:H3B	2.01	0.43
1:D:292:VAL:HG13	2:D:401:FAD:H5'2	2.00	0.43
1:G:77:LEU:HG	1:H:152:HIS:ND1	2.34	0.43
1:H:56:LYS:CB	1:H:306:ASN:HB2	2.48	0.43
1:C:5:GLU:OE2	1:C:323:GLN:HG3	2.18	0.43
1:D:295:ALA:HB2	1:D:302:ILE:CG1	2.48	0.43
1:E:292:VAL:HG12	1:E:302:ILE:O	2.19	0.43
1:H:304:ILE:CA	1:H:308:LYS:HD2	2.49	0.43
1:A:209:HIS:O	1:A:211:LYS:HG3	2.19	0.43
1:H:84:VAL:HG13	1:H:89:LEU:HB2	2.01	0.43
1:A:151:ALA:HB1	1:A:175:LEU:HA	2.01	0.42
1:A:74:ASN:O	1:A:78:VAL:HG23	2.19	0.42
1:E:187:ARG:O	1:E:217:ASN:HA	2.19	0.42
1:H:294:ALA:HB3	1:H:302:ILE:HG21	2.01	0.42
1:D:113:LYS:HB3	1:D:113:LYS:HE2	1.85	0.42
1:A:164:GLY:HA3	1:A:186:TYR:CE1	2.55	0.42
1:G:265:ASN:HB3	1:G:268:GLU:H	1.84	0.42
1:F:108:THR:HG22	1:F:108:THR:O	2.20	0.42
1:A:107:PHE:O	1:A:117:GLU:HA	2.20	0.42
1:A:322:LYS:HB2	1:A:322:LYS:HE3	1.57	0.42
1:C:283:ASN:ND2	1:C:284:ILE:HG13	2.33	0.42
1:G:158:ASP:H	1:G:242:ASP:HB2	1.83	0.42
1:C:185:LEU:HD23	1:C:215:GLU:HB2	2.01	0.42
1:G:149:LYS:HA	1:G:149:LYS:HD2	1.89	0.42
1:H:166:ASN:ND2	1:H:196:LYS:HG2	2.35	0.42
1:H:79:TYR:O	1:H:83:VAL:HG23	2.20	0.42
1:A:281:GLU:OE2	1:A:321:LYS:NZ	2.52	0.42
1:D:120:PHE:HB3	1:D:318:MET:CE	2.50	0.42
1:D:137:GLU:CD	1:D:222:GLN:HE21	2.20	0.42
1:E:276:ASN:O	1:E:278:GLU:N	2.53	0.42
1:G:8:ILE:O	1:G:31:ILE:HA	2.20	0.42
1:B:320:ALA:O	1:B:322:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ARG:HH22	1:C:323:GLN:HB3	1.82	0.42
1:G:127:TYR:CE2	1:G:292:VAL:HB	2.55	0.42
1:G:34:LYS:HB2	2:G:401:FAD:H1B	2.02	0.42
1:H:288:TYR:CD2	1:H:314:ILE:HG23	2.55	0.42
1:A:102:LYS:HG2	1:A:107:PHE:CE1	2.54	0.42
1:A:100:VAL:HG13	1:A:109:ILE:HD13	2.01	0.42
1:A:177:LYS:NZ	1:C:66:VAL:O	2.37	0.42
1:C:268:GLU:HG3	1:E:132:ASN:ND2	2.34	0.42
1:H:43:ASN:HA	1:H:149:LYS:NZ	2.35	0.42
1:C:78:VAL:HG22	1:C:81:ARG:NH2	2.35	0.41
1:H:127:TYR:O	1:H:127:TYR:HD1	2.03	0.41
1:H:217:ASN:ND2	1:H:217:ASN:O	2.48	0.41
1:F:36:ASN:O	1:F:39:GLU:HG2	2.20	0.41
1:A:303:PHE:N	1:A:306:ASN:OD1	2.45	0.41
1:B:265:ASN:OD1	1:B:267:ASN:ND2	2.53	0.41
1:B:276:ASN:ND2	1:B:276:ASN:O	2.28	0.41
1:F:8:ILE:HG12	1:F:122:THR:HB	2.02	0.41
1:E:45:PRO:HG2	1:E:48:GLN:HE21	1.85	0.41
1:G:94:PHE:HZ	1:H:243:TYR:OH	2.04	0.41
1:B:281:GLU:CD	1:B:321:LYS:HZ1	2.23	0.41
1:F:109:ILE:HB	1:F:116:TYR:HB2	2.02	0.41
1:F:164:GLY:HA3	1:F:186:TYR:CE1	2.55	0.41
1:G:217:ASN:O	1:G:232:VAL:HA	2.20	0.41
1:G:30:LEU:HD21	1:G:32:ILE:HD11	2.02	0.41
1:H:279:THR:HA	1:H:313:ILE:HG22	2.03	0.41
1:D:186:TYR:OH	3:D:402[A]:NAP:O1X	2.38	0.41
1:E:265:ASN:O	1:E:271:THR:HA	2.20	0.41
1:G:3:LYS:HA	1:G:117:GLU:O	2.20	0.41
1:G:9:ILE:HD12	1:G:123:ILE:HG12	2.01	0.41
1:H:10:GLY:O	1:H:15:GLY:HA3	2.21	0.41
1:H:68:GLU:O	1:H:68:GLU:HG2	2.20	0.41
1:F:298:ASP:C	1:F:300:ASN:H	2.24	0.41
1:G:138:GLY:HA3	1:G:223:ILE:O	2.21	0.41
1:D:166:ASN:HB2	3:D:402[A]:NAP:H3D	2.02	0.41
1:D:248:ILE:HA	3:D:402[A]:NAP:H51A	2.03	0.41
1:H:304:ILE:H	1:H:308:LYS:HD2	1.85	0.41
1:H:307:GLY:O	1:H:309:PHE:N	2.53	0.41
1:G:19:ALA:HB2	1:G:31:ILE:HD11	2.03	0.41
1:G:34:LYS:HB2	2:G:401:FAD:N3A	2.35	0.41
1:C:102:LYS:HD3	1:C:107:PHE:CE1	2.55	0.40
1:H:51:PHE:HB3	2:H:401:FAD:O4	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320:ALA:O	1:E:322:LYS:HG3	2.21	0.40
1:A:92:ASN:HB3	1:A:95:GLU:OE1	2.21	0.40
2:C:401:FAD:O2'	2:C:401:FAD:O4'	2.26	0.40
1:G:264:ILE:HG22	1:G:265:ASN:H	1.87	0.40
1:G:279:THR:O	1:G:280:TYR:HB2	2.22	0.40
1:H:13:PRO:HD2	2:H:401:FAD:O1A	2.21	0.40
1:A:268:GLU:O	1:A:269:PHE:CB	2.69	0.40
1:C:258:LYS:O	1:C:261:GLY:N	2.46	0.40
1:D:306:ASN:N	1:D:306:ASN:OD1	2.47	0.40
1:E:138:GLY:HA3	1:E:223:ILE:O	2.21	0.40
1:F:151:ALA:HB1	1:F:175:LEU:HA	2.04	0.40
1:D:167:SER:HB3	1:D:247:MET:CE	2.51	0.40
1:D:165:LYS:CD	3:D:402[B]:NAP:H3B	2.50	0.40
1:D:7:ILE:HD13	1:D:7:ILE:HG21	1.86	0.40
1:G:4:VAL:O	1:G:118:CYS:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	321/328 (98%)	303 (94%)	17 (5%)	1 (0%)	41 71
1	B	321/328 (98%)	296 (92%)	22 (7%)	3 (1%)	17 48
1	C	322/328 (98%)	305 (95%)	16 (5%)	1 (0%)	41 71
1	D	322/328 (98%)	307 (95%)	11 (3%)	4 (1%)	13 40
1	E	322/328 (98%)	301 (94%)	20 (6%)	1 (0%)	41 71
1	F	323/328 (98%)	300 (93%)	18 (6%)	5 (2%)	10 34
1	G	261/328 (80%)	220 (84%)	34 (13%)	7 (3%)	5 19
1	H	321/328 (98%)	278 (87%)	27 (8%)	16 (5%)	2 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2513/2624 (96%)	2310 (92%)	165 (7%)	38 (2%)	10 34

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	ASP
1	C	271	THR
1	D	277	LYS
1	D	298	ASP
1	E	277	LYS
1	F	61	ASP
1	F	277	LYS
1	G	63	PRO
1	G	69	SER
1	H	166	ASN
1	H	217	ASN
1	H	277	LYS
1	H	312	GLY
1	D	266	THR
1	F	60	GLY
1	F	298	ASP
1	G	296	GLY
1	H	165	LYS
1	H	264	ILE
1	H	304	ILE
1	B	266	THR
1	D	300	ASN
1	G	67	GLU
1	H	50	PHE
1	H	53	SER
1	H	63	PRO
1	H	72	ARG
1	A	269	PHE
1	G	74	ASN
1	G	270	GLY
1	H	298	ASP
1	H	299	ALA
1	H	309	PHE
1	F	266	THR
1	H	297	ASN
1	H	305	GLU
1	G	71	PRO

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Mol	Chain	Res	Type
1	B	264	ILE

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	277/282 (98%)	264 (95%)	13 (5%)	26	59
1	B	277/282 (98%)	268 (97%)	9 (3%)	39	73
1	C	278/282 (99%)	270 (97%)	8 (3%)	42	76
1	D	278/282 (99%)	268 (96%)	10 (4%)	35	69
1	E	278/282 (99%)	268 (96%)	10 (4%)	35	69
1	F	279/282 (99%)	271 (97%)	8 (3%)	42	76
1	G	230/282 (82%)	217 (94%)	13 (6%)	20	51
1	H	277/282 (98%)	258 (93%)	19 (7%)	15	41
All	All	2174/2256 (96%)	2084 (96%)	90 (4%)	30	64

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	PHE
1	A	99	THR
1	A	108	THR
1	A	133	THR
1	A	136	VAL
1	A	156	ASP
1	A	204	THR
1	A	265	ASN
1	A	266	THR
1	A	268	GLU
1	A	271	THR
1	A	274	MET
1	A	293	ILE
1	B	127	TYR

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Mol	Chain	Res	Type
1	B	133	THR
1	B	156	ASP
1	B	204	THR
1	B	265	ASN
1	B	266	THR
1	B	274	MET
1	B	276	ASN
1	B	301	THR
1	C	1	MET
1	C	64	PHE
1	C	99	THR
1	C	108	THR
1	C	127	TYR
1	C	133	THR
1	C	156	ASP
1	C	303	PHE
1	D	64	PHE
1	D	103	MET
1	D	127	TYR
1	D	133	THR
1	D	156	ASP
1	D	207	VAL
1	D	260	VAL
1	D	265	ASN
1	D	301	THR
1	D	303	PHE
1	E	99	THR
1	E	127	TYR
1	E	133	THR
1	E	156	ASP
1	E	204	THR
1	E	260	VAL
1	E	266	THR
1	E	268	GLU
1	E	301	THR
1	E	303	PHE
1	F	64	PHE
1	F	108	THR
1	F	127	TYR
1	F	156	ASP
1	F	200	LEU
1	F	260	VAL

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Mol	Chain	Res	Type
1	F	265	ASN
1	F	303	PHE
1	G	4	VAL
1	G	29	THR
1	G	37	VAL
1	G	62	VAL
1	G	66	VAL
1	G	72	ARG
1	G	95	GLU
1	G	122	THR
1	G	156	ASP
1	G	158	ASP
1	G	265	ASN
1	G	303	PHE
1	G	313	ILE
1	H	28	ASP
1	H	37	VAL
1	H	53	SER
1	H	55	ASP
1	H	73	ARG
1	H	74	ASN
1	H	108	THR
1	H	127	TYR
1	H	156	ASP
1	H	212	ILE
1	H	217	ASN
1	H	260	VAL
1	H	266	THR
1	H	301	THR
1	H	303	PHE
1	H	305	GLU
1	H	306	ASN
1	H	309	PHE
1	H	310	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	B	267	ASN
1	D	74	ASN
1	D	297	ASN

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Mol	Chain	Res	Type
1	E	48	GLN
1	F	300	ASN
1	G	276	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

12 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	NAP	D	402[B]	-	45,52,52	0.97	3 (6%)	56,80,80	1.12	4 (7%)
3	NAP	F	402	-	45,52,52	1.20	4 (8%)	56,80,80	1.26	7 (12%)
2	FAD	B	401	-	51,58,58	1.27	5 (9%)	60,89,89	2.31	9 (15%)
3	NAP	C	402	-	45,52,52	1.21	5 (11%)	56,80,80	1.24	7 (12%)
2	FAD	C	401	-	51,58,58	1.25	5 (9%)	60,89,89	2.32	8 (13%)
2	FAD	F	401	-	51,58,58	1.26	6 (11%)	60,89,89	2.24	7 (11%)
2	FAD	A	401	-	51,58,58	1.28	5 (9%)	60,89,89	2.32	9 (15%)
2	FAD	D	401	-	51,58,58	1.19	3 (5%)	60,89,89	2.26	7 (11%)
2	FAD	G	401	-	51,58,58	1.17	4 (7%)	60,89,89	2.23	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FAD	E	401	-	51,58,58	1.33	4 (7%)	60,89,89	2.24	6 (10%)
2	FAD	H	401	-	51,58,58	1.23	4 (7%)	60,89,89	2.31	8 (13%)
3	NAP	D	402[A]	-	45,52,52	0.93	3 (6%)	56,80,80	1.08	3 (5%)

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	NAP	D	402[B]	-	-	16/31/67/67	0/5/5/5
3	NAP	F	402	-	-	17/31/67/67	0/5/5/5
2	FAD	B	401	-	-	5/30/50/50	0/6/6/6
3	NAP	C	402	-	-	17/31/67/67	0/5/5/5
2	FAD	C	401	-	-	1/30/50/50	0/6/6/6
2	FAD	F	401	-	-	4/30/50/50	0/6/6/6
2	FAD	A	401	-	-	9/30/50/50	0/6/6/6
2	FAD	D	401	-	-	8/30/50/50	0/6/6/6
2	FAD	G	401	-	-	4/30/50/50	0/6/6/6
2	FAD	E	401	-	-	7/30/50/50	0/6/6/6
2	FAD	H	401	-	-	7/30/50/50	0/6/6/6
3	NAP	D	402[A]	-	-	13/31/67/67	0/5/5/5

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	FAD	C4X-C10	5.69	1.44	1.38
2	E	401	FAD	C4X-C10	5.51	1.44	1.38
2	C	401	FAD	C4X-C10	5.49	1.44	1.38
2	F	401	FAD	C4X-C10	5.36	1.44	1.38
2	A	401	FAD	C4X-C10	5.33	1.44	1.38
2	H	401	FAD	C4X-C10	5.30	1.44	1.38
2	D	401	FAD	C4X-C10	5.29	1.44	1.38
2	G	401	FAD	C4X-C10	5.18	1.44	1.38
2	H	401	FAD	C4-N3	3.74	1.39	1.33
2	E	401	FAD	C5X-N5	3.71	1.41	1.35
2	E	401	FAD	C4-N3	3.40	1.39	1.33
2	A	401	FAD	C4-N3	3.34	1.38	1.33
3	C	402	NAP	C5A-C4A	3.33	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	FAD	C4-N3	3.29	1.38	1.33
3	F	402	NAP	O4B-C1B	3.29	1.45	1.41
2	F	401	FAD	C4-N3	3.28	1.38	1.33
3	F	402	NAP	C5A-C4A	3.14	1.49	1.40
3	C	402	NAP	O4B-C1B	3.12	1.45	1.41
3	C	402	NAP	O4D-C1D	3.07	1.45	1.41
2	C	401	FAD	C4-N3	3.02	1.38	1.33
3	F	402	NAP	O4D-C1D	2.90	1.45	1.41
2	E	401	FAD	C4-C4X	2.83	1.46	1.41
2	A	401	FAD	C4-C4X	2.78	1.46	1.41
3	D	402[B]	NAP	O4B-C1B	2.77	1.44	1.41
3	D	402[A]	NAP	C5A-C4A	2.71	1.48	1.40
3	D	402[B]	NAP	C5A-C4A	2.69	1.48	1.40
2	D	401	FAD	C5X-N5	2.67	1.39	1.35
3	C	402	NAP	C2A-N3A	2.66	1.36	1.32
2	F	401	FAD	C4-C4X	2.63	1.45	1.41
2	B	401	FAD	C4X-N5	-2.58	1.29	1.33
2	H	401	FAD	C9A-N10	2.57	1.42	1.38
2	G	401	FAD	C4X-N5	-2.55	1.29	1.33
2	C	401	FAD	C5X-N5	2.48	1.39	1.35
2	A	401	FAD	P-O2P	-2.44	1.43	1.55
2	G	401	FAD	C4-C4X	2.40	1.45	1.41
2	G	401	FAD	C4-N3	2.38	1.37	1.33
2	A	401	FAD	C5X-N5	2.32	1.39	1.35
2	C	401	FAD	P-O2P	-2.28	1.44	1.55
2	C	401	FAD	C4-C4X	2.28	1.45	1.41
3	D	402[A]	NAP	O4B-C1B	2.26	1.44	1.41
2	B	401	FAD	C5X-N5	2.25	1.39	1.35
2	D	401	FAD	C4-N3	2.22	1.36	1.33
2	B	401	FAD	C9A-N10	2.22	1.41	1.38
2	F	401	FAD	P-O2P	-2.18	1.45	1.55
3	F	402	NAP	C2A-N3A	2.18	1.35	1.32
3	D	402[B]	NAP	C2A-N3A	2.17	1.35	1.32
3	C	402	NAP	P2B-O2B	2.14	1.63	1.59
2	H	401	FAD	C5X-N5	2.13	1.38	1.35
2	F	401	FAD	C9A-N10	2.12	1.41	1.38
2	F	401	FAD	C5X-N5	2.09	1.38	1.35
3	D	402[A]	NAP	O4D-C1D	2.06	1.44	1.41

All (82) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	FAD	C4-N3-C2	13.38	126.44	115.14
2	A	401	FAD	C4-N3-C2	13.27	126.34	115.14
2	C	401	FAD	C4-N3-C2	13.24	126.32	115.14
2	F	401	FAD	C4-N3-C2	13.21	126.29	115.14
2	E	401	FAD	C4-N3-C2	13.19	126.28	115.14
2	B	401	FAD	C4-N3-C2	13.09	126.19	115.14
2	H	401	FAD	C4-N3-C2	12.95	126.08	115.14
2	G	401	FAD	C4-N3-C2	12.89	126.02	115.14
2	A	401	FAD	C4X-C4-N3	-7.30	113.45	123.43
2	F	401	FAD	C4X-C4-N3	-7.13	113.68	123.43
2	E	401	FAD	C4X-C4-N3	-6.97	113.90	123.43
2	G	401	FAD	C4X-C4-N3	-6.93	113.95	123.43
2	C	401	FAD	C4X-C4-N3	-6.86	114.05	123.43
2	B	401	FAD	C4X-C4-N3	-6.81	114.11	123.43
2	D	401	FAD	C4X-C4-N3	-6.76	114.18	123.43
2	H	401	FAD	C4X-C4-N3	-6.75	114.19	123.43
2	B	401	FAD	C10-C4X-N5	5.10	124.78	121.26
2	H	401	FAD	C10-C4X-N5	5.07	124.77	121.26
2	G	401	FAD	C10-C4X-N5	4.79	124.57	121.26
2	D	401	FAD	C10-C4X-N5	4.66	124.48	121.26
2	C	401	FAD	C10-C4X-N5	4.59	124.44	121.26
2	F	401	FAD	C10-C4X-N5	4.36	124.28	121.26
2	E	401	FAD	C10-C4X-N5	4.22	124.18	121.26
2	A	401	FAD	C10-C4X-N5	4.18	124.15	121.26
2	H	401	FAD	C4-C4X-C10	-4.08	117.25	119.95
2	C	401	FAD	C4-C4X-C10	-4.02	117.29	119.95
2	D	401	FAD	C4-C4X-C10	-3.97	117.32	119.95
2	E	401	FAD	C4-C4X-C10	-3.94	117.34	119.95
2	A	401	FAD	C4-C4X-C10	-3.92	117.35	119.95
2	G	401	FAD	C4-C4X-C10	-3.87	117.39	119.95
2	C	401	FAD	P-O3P-PA	-3.86	119.60	132.83
2	H	401	FAD	C1'-N10-C9A	3.83	121.31	118.29
2	F	401	FAD	C4X-C10-N10	-3.80	116.40	120.30
2	B	401	FAD	C4-C4X-C10	-3.72	117.49	119.95
2	B	401	FAD	C4X-C10-N10	-3.69	116.51	120.30
2	H	401	FAD	C4X-C10-N10	-3.57	116.64	120.30
2	C	401	FAD	C4X-C10-N10	-3.56	116.64	120.30
2	D	401	FAD	C4X-C10-N10	-3.51	116.69	120.30
2	F	401	FAD	C4-C4X-C10	-3.48	117.64	119.95
2	G	401	FAD	C4X-C10-N10	-3.43	116.77	120.30
2	A	401	FAD	C4X-C10-N10	-3.42	116.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	FAD	C4X-C10-N10	-3.37	116.84	120.30
2	H	401	FAD	P-O3P-PA	-3.34	121.38	132.83
3	D	402[A]	NAP	N3A-C2A-N1A	-3.28	123.56	128.68
2	G	401	FAD	C1'-N10-C9A	3.16	120.78	118.29
3	D	402[B]	NAP	N3A-C2A-N1A	-3.12	123.80	128.68
2	B	401	FAD	C4'-C3'-C2'	-3.11	106.89	113.36
3	D	402[B]	NAP	PN-O3-PA	-3.08	122.25	132.83
2	A	401	FAD	C1'-N10-C9A	3.01	120.66	118.29
3	C	402	NAP	N3A-C2A-N1A	-2.96	124.05	128.68
3	F	402	NAP	N3A-C2A-N1A	-2.96	124.06	128.68
3	D	402[B]	NAP	C4A-C5A-N7A	-2.92	106.35	109.40
2	A	401	FAD	O5'-P-O1P	-2.91	97.69	109.07
3	D	402[A]	NAP	C4A-C5A-N7A	-2.86	106.42	109.40
3	D	402[A]	NAP	C3D-C2D-C1D	2.85	105.26	100.98
3	C	402	NAP	O7N-C7N-C3N	-2.82	116.26	119.63
3	F	402	NAP	C3D-C2D-C1D	2.73	105.08	100.98
2	B	401	FAD	C1'-N10-C9A	2.72	120.44	118.29
2	D	401	FAD	C1'-N10-C9A	2.70	120.42	118.29
2	C	401	FAD	C1'-N10-C9A	2.69	120.41	118.29
2	F	401	FAD	C1'-N10-C9A	2.60	120.34	118.29
2	C	401	FAD	C5A-C6A-N6A	2.58	124.27	120.35
2	D	401	FAD	C5A-C6A-N6A	2.52	124.19	120.35
2	E	401	FAD	C5A-C6A-N6A	2.51	124.17	120.35
3	F	402	NAP	C2B-C3B-C4B	2.48	107.38	101.99
3	C	402	NAP	C3N-C7N-N7N	2.47	120.71	117.75
2	F	401	FAD	C5A-C6A-N6A	2.44	124.05	120.35
2	B	401	FAD	C5A-C6A-N6A	2.38	123.97	120.35
2	B	401	FAD	C5'-C4'-C3'	2.33	116.70	112.20
2	H	401	FAD	C5A-C6A-N6A	2.24	123.76	120.35
3	C	402	NAP	C4A-C5A-N7A	-2.24	107.07	109.40
3	C	402	NAP	PN-O3-PA	-2.19	125.30	132.83
3	F	402	NAP	O5D-C5D-C4D	2.18	116.48	108.99
2	A	401	FAD	P-O3P-PA	-2.17	125.38	132.83
3	C	402	NAP	O3X-P2B-O2X	2.15	115.84	107.64
3	C	402	NAP	N6A-C6A-N1A	2.11	122.96	118.57
3	F	402	NAP	O2B-P2B-O1X	-2.10	101.28	109.39
3	D	402[B]	NAP	O4D-C1D-C2D	-2.10	103.86	106.93
3	F	402	NAP	C2D-C3D-C4D	2.09	106.70	102.64
2	G	401	FAD	C5A-C6A-N6A	2.09	123.53	120.35
3	F	402	NAP	PN-O3-PA	-2.08	125.68	132.83
2	A	401	FAD	C5A-C6A-N6A	2.02	123.42	120.35

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	402[B]	NAP	C5B-O5B-PA-O1A
3	D	402[B]	NAP	C5B-O5B-PA-O2A
3	D	402[B]	NAP	O4B-C4B-C5B-O5B
3	D	402[B]	NAP	C3B-C4B-C5B-O5B
3	D	402[B]	NAP	C5D-O5D-PN-O3
3	D	402[B]	NAP	C5D-O5D-PN-O1N
3	D	402[B]	NAP	C5D-O5D-PN-O2N
3	D	402[B]	NAP	O4D-C4D-C5D-O5D
3	D	402[B]	NAP	C2N-C3N-C7N-O7N
3	D	402[B]	NAP	C2N-C3N-C7N-N7N
3	F	402	NAP	C5B-O5B-PA-O3
3	F	402	NAP	C3B-C4B-C5B-O5B
3	F	402	NAP	C5D-O5D-PN-O3
3	F	402	NAP	C5D-O5D-PN-O1N
3	F	402	NAP	C5D-O5D-PN-O2N
3	F	402	NAP	C2N-C3N-C7N-O7N
3	F	402	NAP	C2N-C3N-C7N-N7N
3	F	402	NAP	C4N-C3N-C7N-N7N
3	C	402	NAP	C5B-O5B-PA-O2A
3	C	402	NAP	C5D-O5D-PN-O3
3	C	402	NAP	C2N-C3N-C7N-N7N
2	A	401	FAD	C5B-O5B-PA-O2A
2	A	401	FAD	C5B-O5B-PA-O3P
2	A	401	FAD	C5'-O5'-P-O1P
2	A	401	FAD	C5'-O5'-P-O2P
2	D	401	FAD	C5B-O5B-PA-O1A
2	D	401	FAD	C5B-O5B-PA-O2A
2	G	401	FAD	PA-O3P-P-O5'
2	H	401	FAD	C3'-C4'-C5'-O5'
2	H	401	FAD	O4'-C4'-C5'-O5'
3	D	402[A]	NAP	C5B-O5B-PA-O3
3	D	402[A]	NAP	O4B-C4B-C5B-O5B
3	D	402[A]	NAP	O4D-C4D-C5D-O5D
3	F	402	NAP	C4N-C3N-C7N-O7N
3	D	402[B]	NAP	C4N-C3N-C7N-O7N
3	D	402[B]	NAP	C4N-C3N-C7N-N7N
3	C	402	NAP	C4N-C3N-C7N-N7N
3	C	402	NAP	C4N-C3N-C7N-O7N
3	C	402	NAP	C2N-C3N-C7N-O7N
2	H	401	FAD	O3'-C3'-C4'-O4'
3	D	402[B]	NAP	C3D-C4D-C5D-O5D
3	F	402	NAP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	A	401	FAD	O4B-C4B-C5B-O5B
2	D	401	FAD	O4B-C4B-C5B-O5B
2	D	401	FAD	C3B-C4B-C5B-O5B
2	H	401	FAD	C2'-C3'-C4'-O4'
2	H	401	FAD	C2'-C3'-C4'-C5'
2	G	401	FAD	O4B-C4B-C5B-O5B
3	D	402[A]	NAP	C3B-C4B-C5B-O5B
3	D	402[A]	NAP	C3D-C4D-C5D-O5D
3	F	402	NAP	C1B-C2B-O2B-P2B
3	F	402	NAP	C3B-C2B-O2B-P2B
3	C	402	NAP	C3B-C2B-O2B-P2B
3	D	402[A]	NAP	C3B-C2B-O2B-P2B
2	H	401	FAD	O3'-C3'-C4'-C5'
3	D	402[A]	NAP	C4D-C5D-O5D-PN
3	D	402[A]	NAP	C1B-C2B-O2B-P2B
2	A	401	FAD	C3B-C4B-C5B-O5B
3	C	402	NAP	O4B-C4B-C5B-O5B
3	F	402	NAP	C4D-C5D-O5D-PN
2	B	401	FAD	PA-O3P-P-O5'
2	F	401	FAD	PA-O3P-P-O5'
2	A	401	FAD	PA-O3P-P-O5'
2	D	401	FAD	P-O3P-PA-O5B
2	E	401	FAD	PA-O3P-P-O5'
3	D	402[B]	NAP	C2B-O2B-P2B-O1X
2	B	401	FAD	C5'-O5'-P-O3P
3	C	402	NAP	C5B-O5B-PA-O3
3	D	402[B]	NAP	PA-O3-PN-O2N
2	B	401	FAD	P-O3P-PA-O1A
3	C	402	NAP	PA-O3-PN-O2N
2	H	401	FAD	C4'-C5'-O5'-P
3	F	402	NAP	C5B-O5B-PA-O1A
3	F	402	NAP	C5B-O5B-PA-O2A
2	B	401	FAD	C5'-O5'-P-O1P
3	C	402	NAP	C5D-O5D-PN-O1N
3	C	402	NAP	C5D-O5D-PN-O2N
2	A	401	FAD	C5B-O5B-PA-O1A
3	D	402[A]	NAP	C5B-O5B-PA-O1A
3	D	402[A]	NAP	C5B-O5B-PA-O2A
2	G	401	FAD	C3B-C4B-C5B-O5B
3	C	402	NAP	C1B-C2B-O2B-P2B
3	C	402	NAP	C3B-C4B-C5B-O5B
2	D	401	FAD	C4B-C5B-O5B-PA

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Mol	Chain	Res	Type	Atoms
2	E	401	FAD	P-O3P-PA-O1A
2	C	401	FAD	O4B-C4B-C5B-O5B
3	F	402	NAP	C2B-O2B-P2B-O1X
3	D	402[A]	NAP	C2B-O2B-P2B-O1X
3	D	402[B]	NAP	C5B-O5B-PA-O3
3	C	402	NAP	C2B-O2B-P2B-O2X
2	A	401	FAD	C5'-O5'-P-O3P
2	D	401	FAD	C5B-O5B-PA-O3P
2	E	401	FAD	C5'-O5'-P-O3P
3	D	402[A]	NAP	C2B-O2B-P2B-O2X
3	D	402[A]	NAP	C2B-O2B-P2B-O3X
2	F	401	FAD	O4B-C4B-C5B-O5B
3	F	402	NAP	PA-O3-PN-O2N
3	C	402	NAP	PA-O3-PN-O1N
2	F	401	FAD	P-O3P-PA-O1A
2	F	401	FAD	P-O3P-PA-O2A
2	D	401	FAD	PA-O3P-P-O1P
2	G	401	FAD	P-O3P-PA-O2A
2	E	401	FAD	P-O3P-PA-O2A
3	C	402	NAP	C5B-O5B-PA-O1A
2	E	401	FAD	C5'-O5'-P-O1P
2	B	401	FAD	O4B-C4B-C5B-O5B
2	E	401	FAD	O4B-C4B-C5B-O5B
2	E	401	FAD	N10-C1'-C2'-O2'

There are no ring outliers.

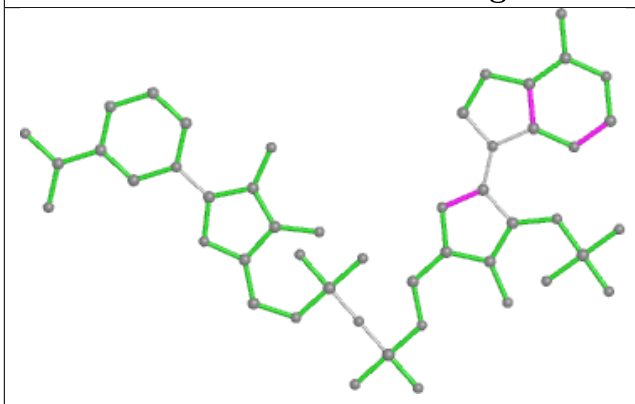
10 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402[B]	NAP	8	0
3	F	402	NAP	6	0
3	C	402	NAP	4	0
2	C	401	FAD	3	0
2	F	401	FAD	2	0
2	A	401	FAD	3	0
2	D	401	FAD	3	0
2	G	401	FAD	5	0
2	H	401	FAD	5	0
3	D	402[A]	NAP	10	0

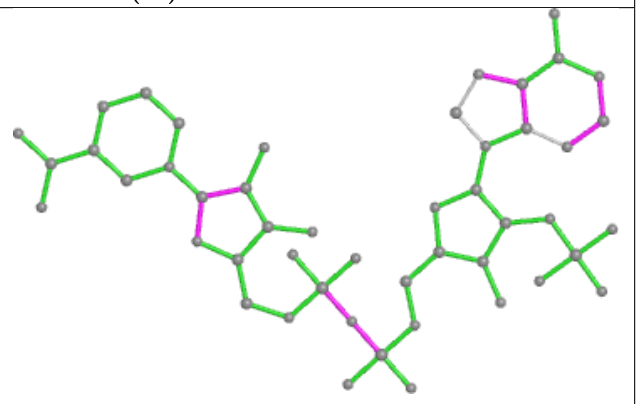
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

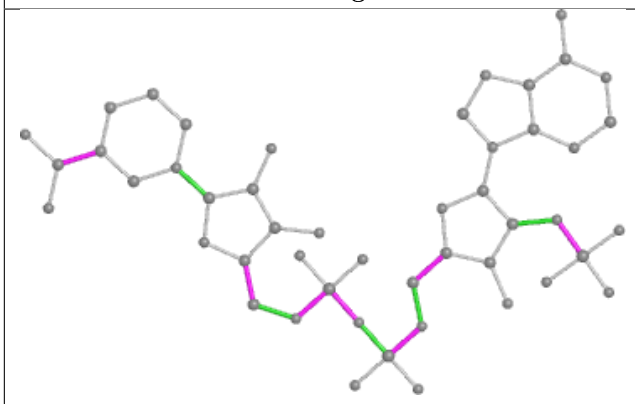
Ligand NAP D 402 (B)



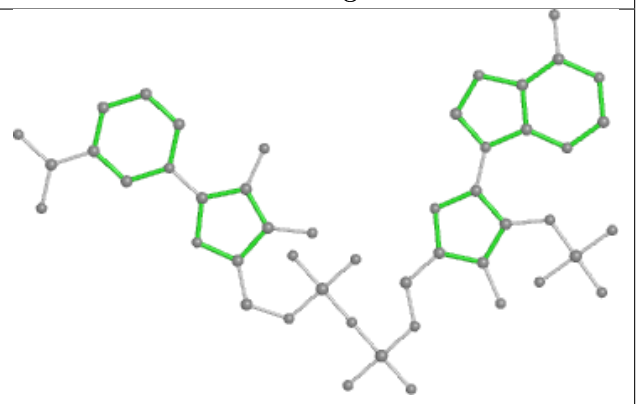
Bond lengths



Bond angles

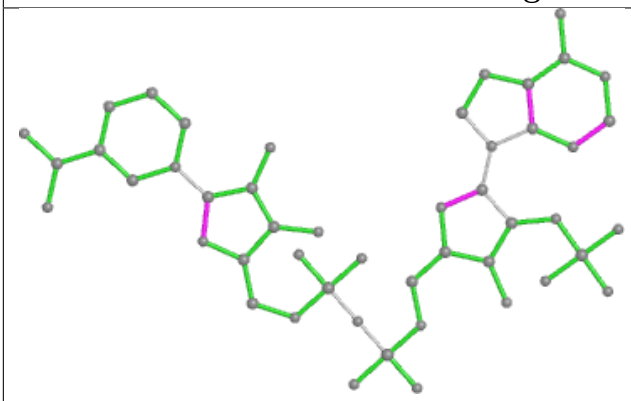


Torsions

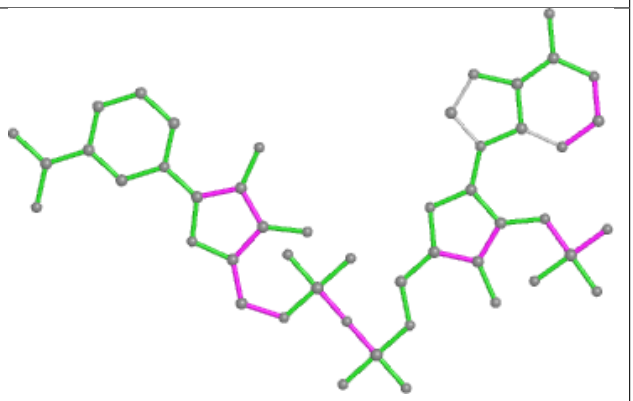


Rings

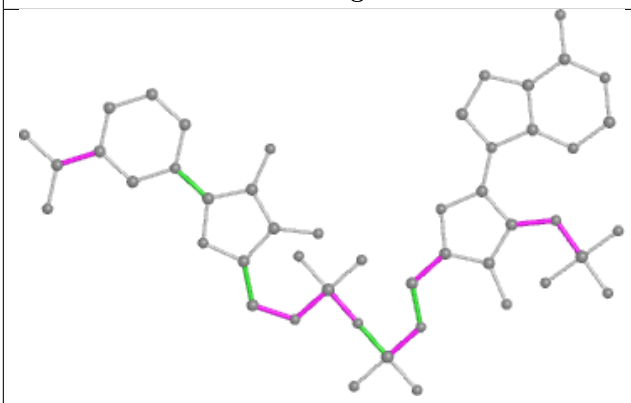
Ligand NAP F 402



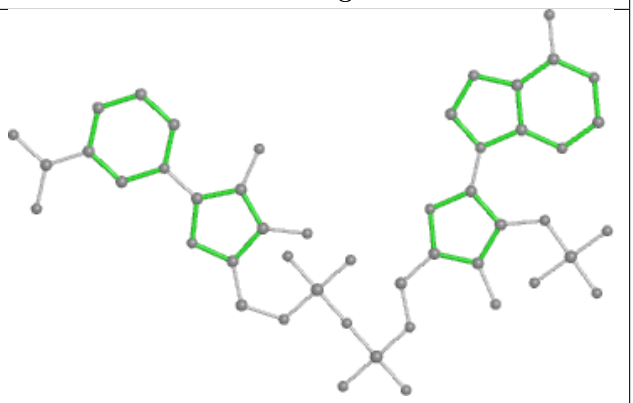
Bond lengths



Bond angles

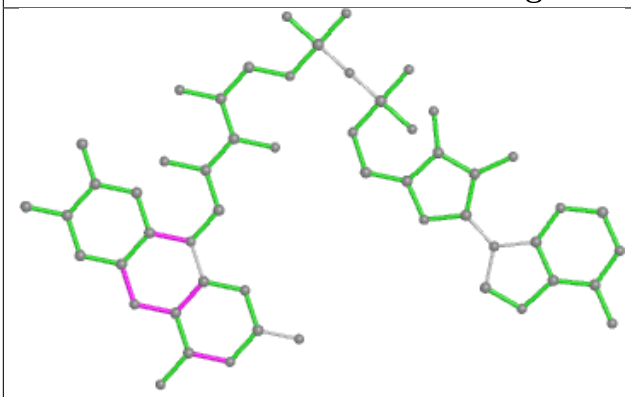


Torsions

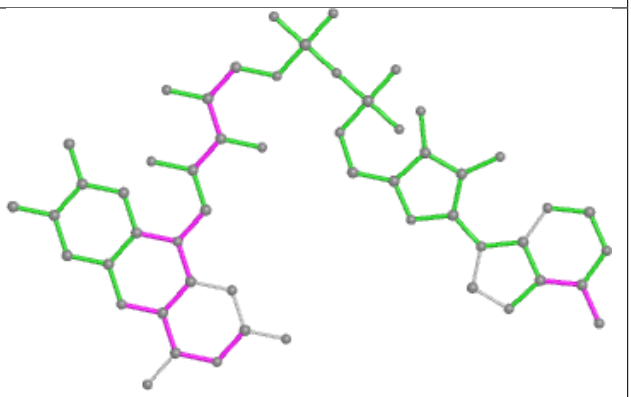


Rings

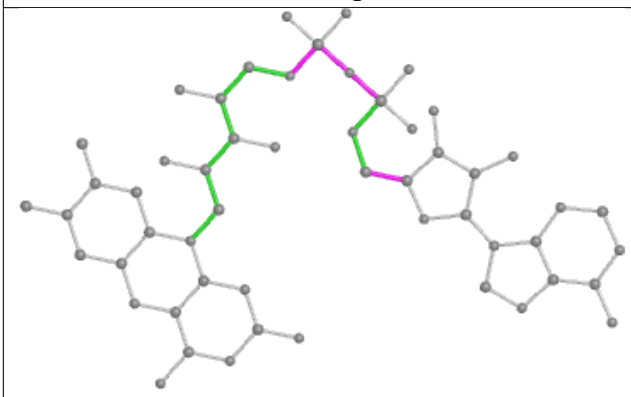
Ligand FAD B 401



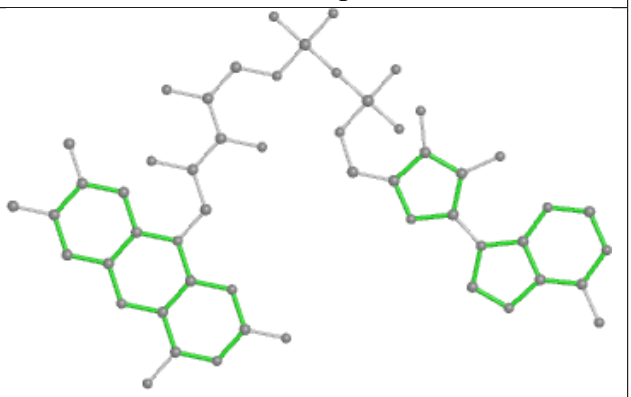
Bond lengths



Bond angles

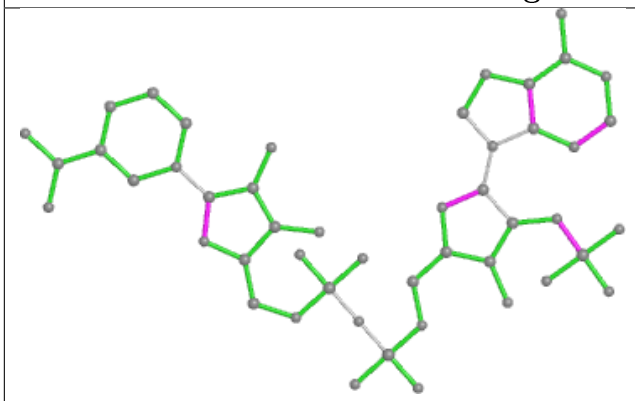


Torsions

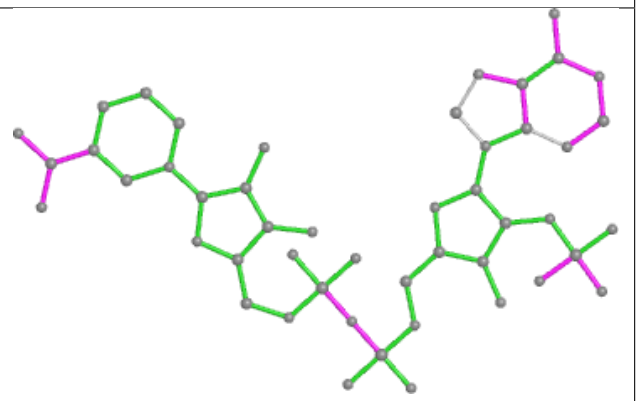


Rings

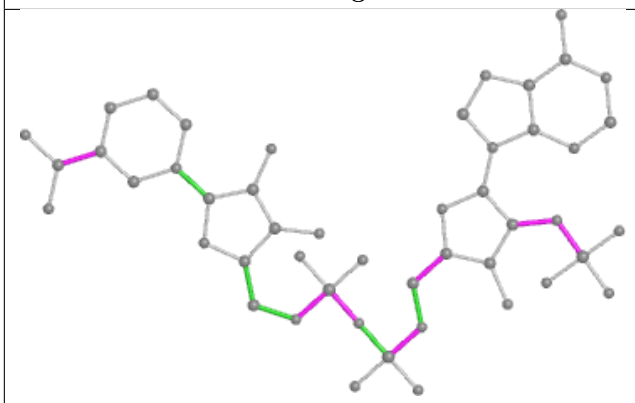
Ligand NAP C 402



Bond lengths



Bond angles



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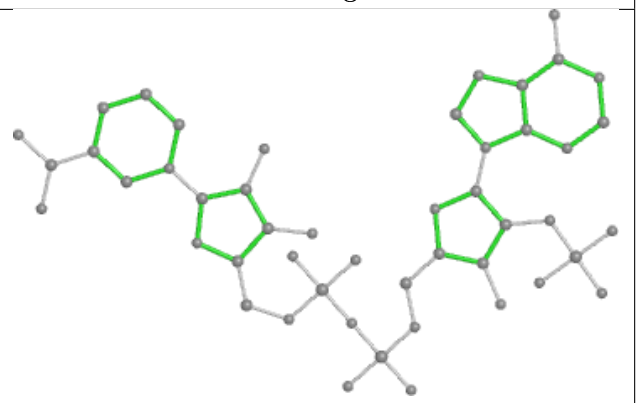
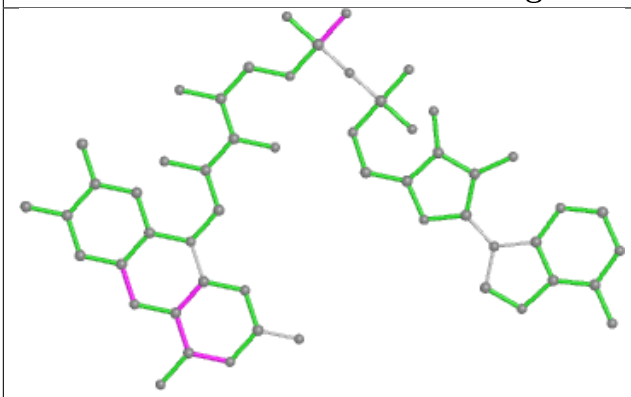
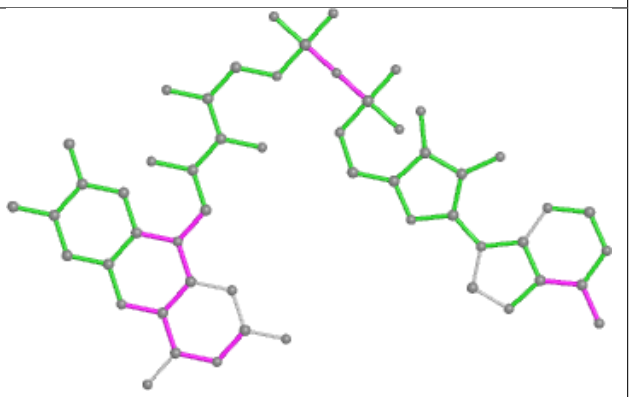


Rings

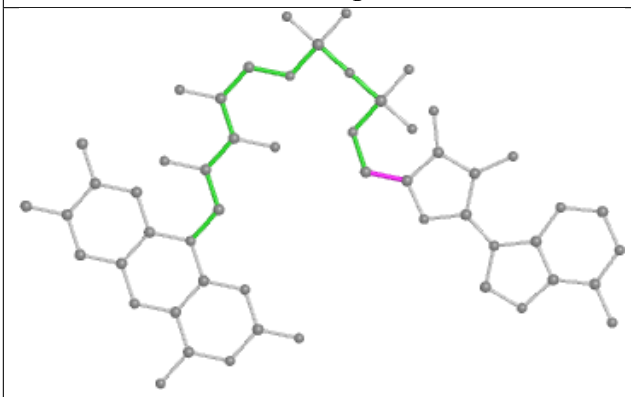
Ligand FAD C 401



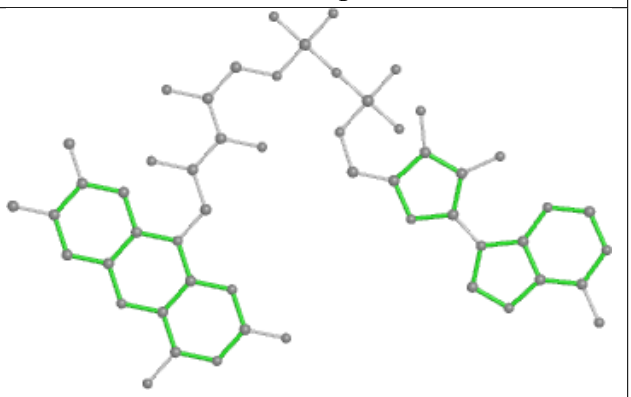
Bond lengths



Bond angles

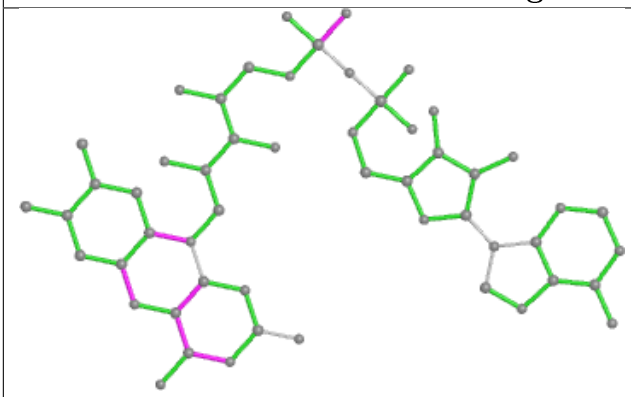


Torsions

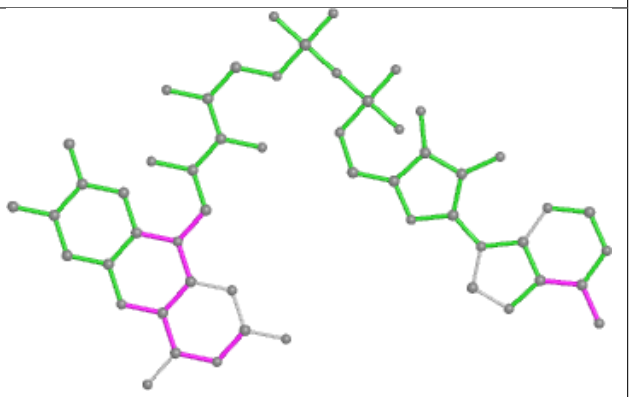


Rings

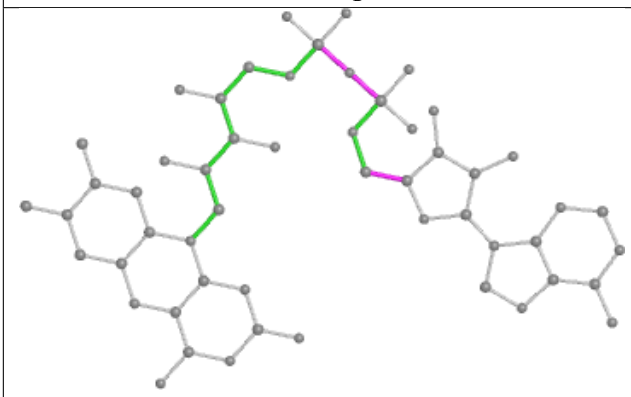
Ligand FAD F 401



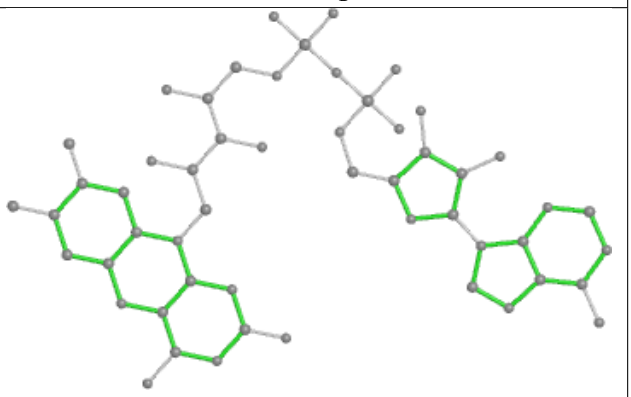
Bond lengths



Bond angles

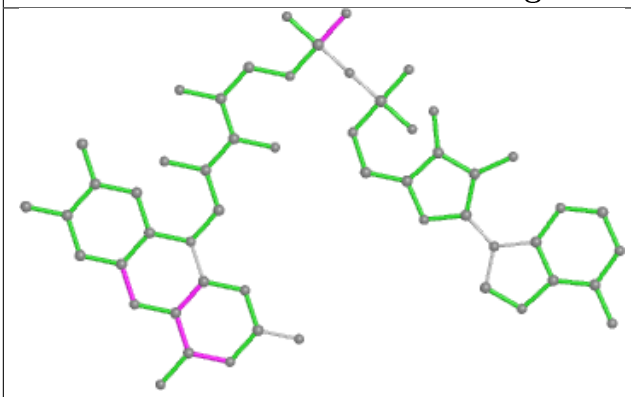


Torsions

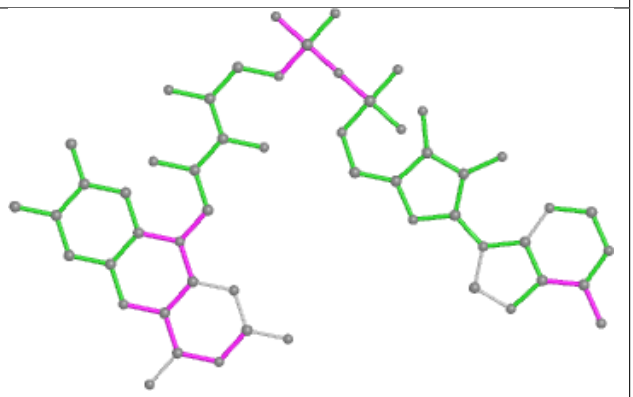


Rings

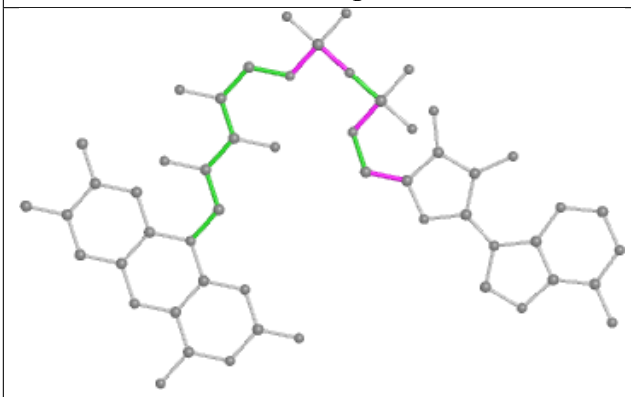
Ligand FAD A 401



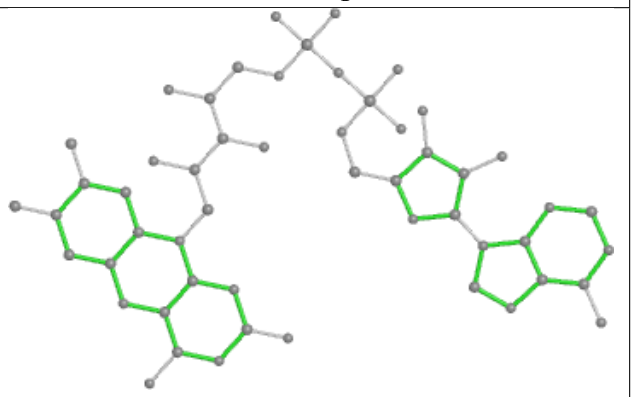
Bond lengths



Bond angles

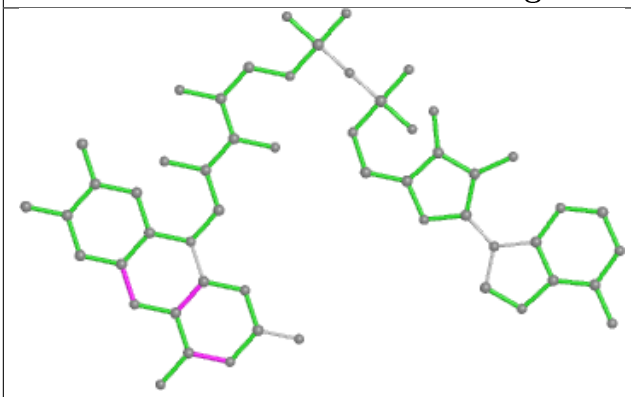


Torsions

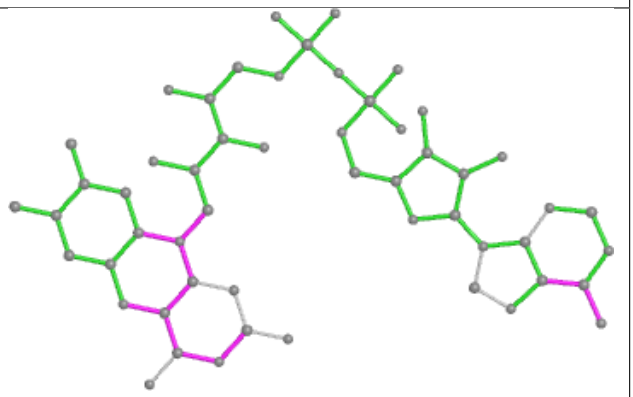


Rings

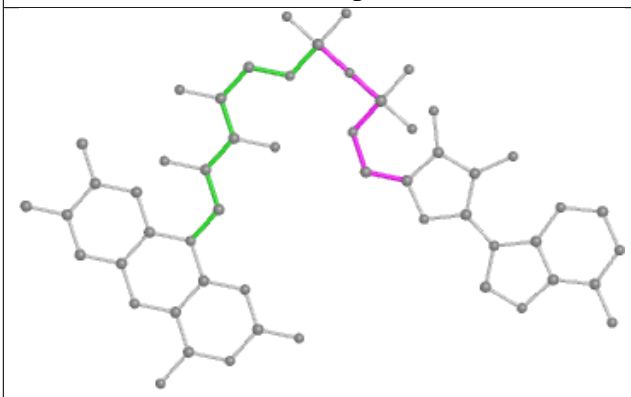
Ligand FAD D 401



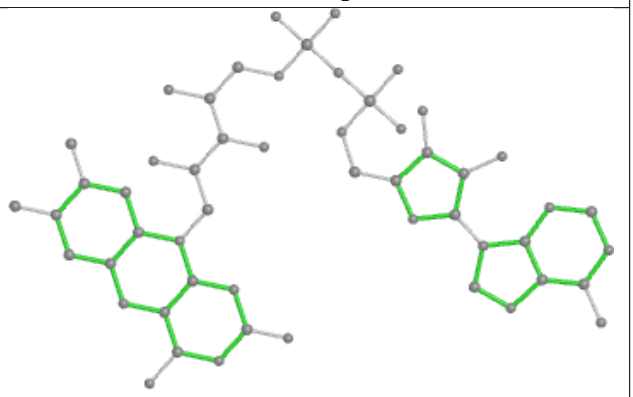
Bond lengths



Bond angles

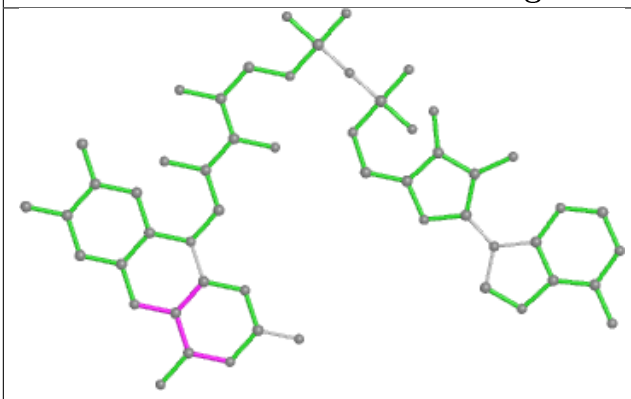


Torsions

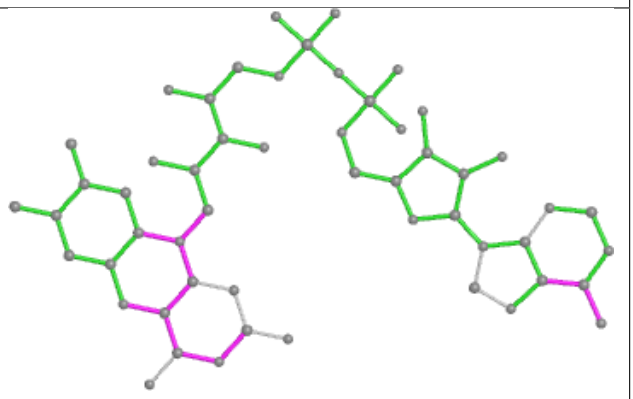


Rings

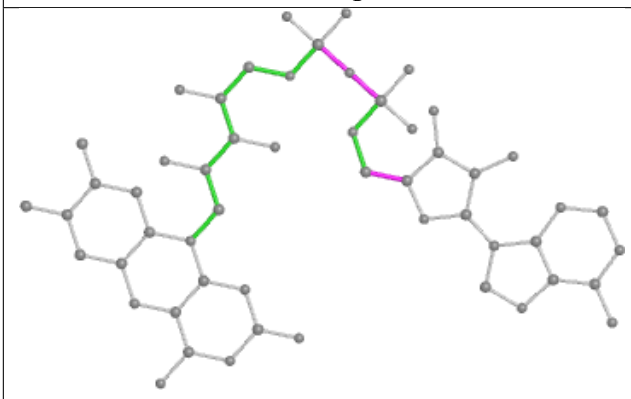
Ligand FAD G 401



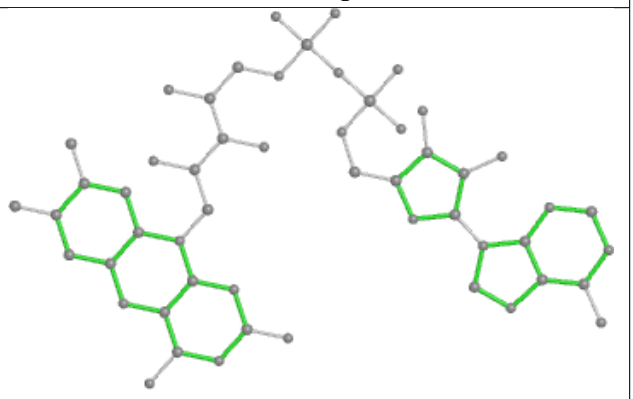
Bond lengths



Bond angles

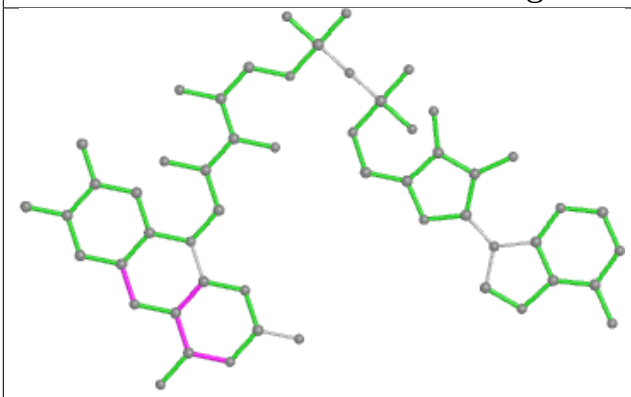


Torsions

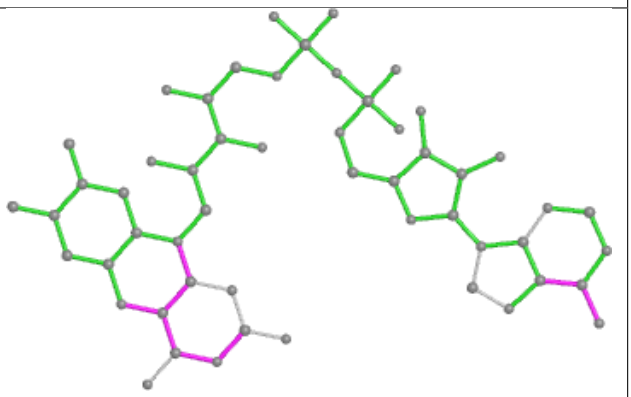


Rings

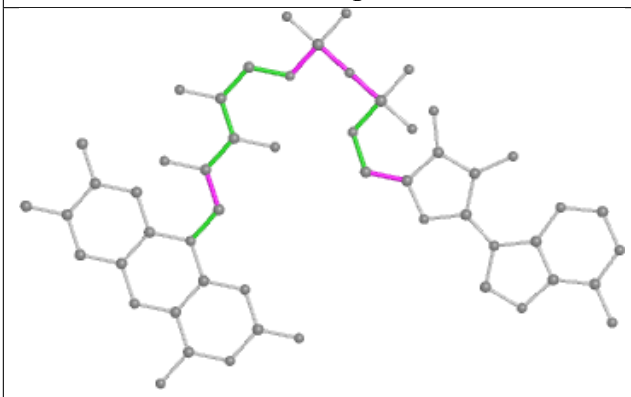
Ligand FAD E 401



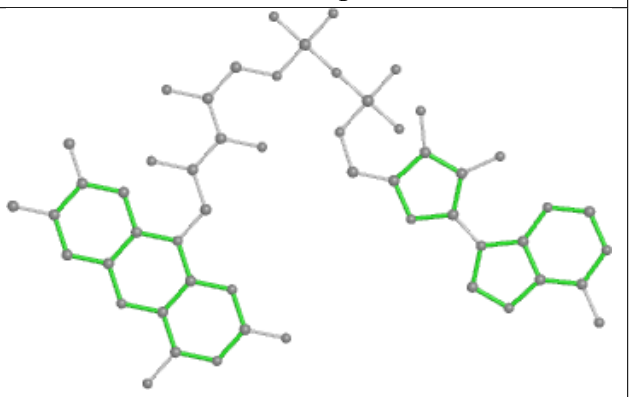
Bond lengths



Bond angles

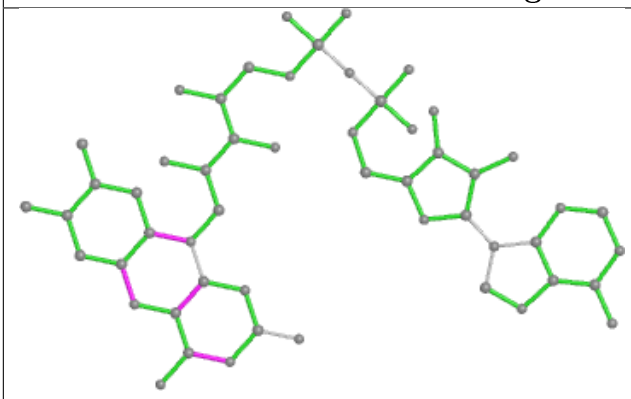


Torsions

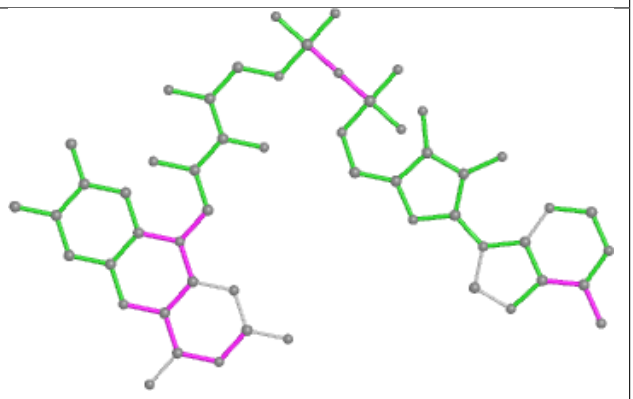


Rings

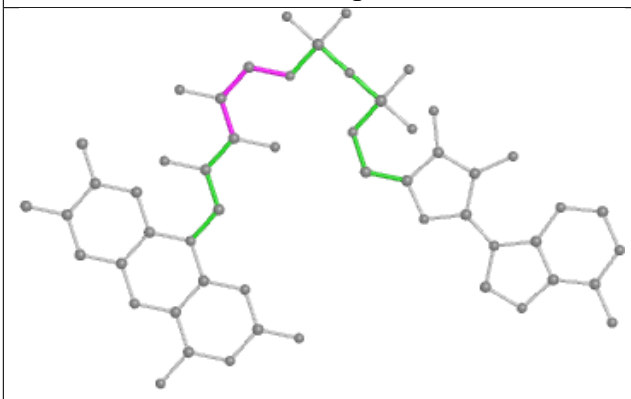
Ligand FAD H 401



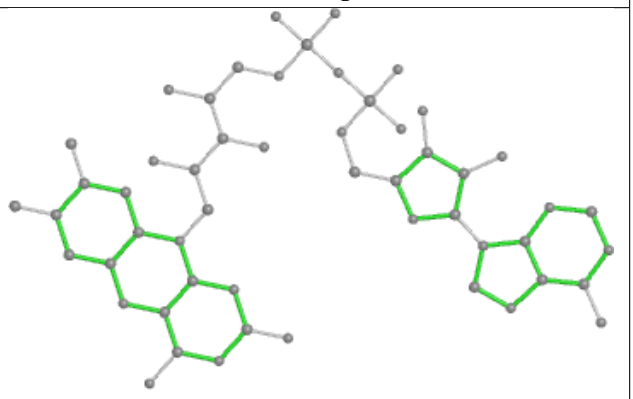
Bond lengths



Bond angles

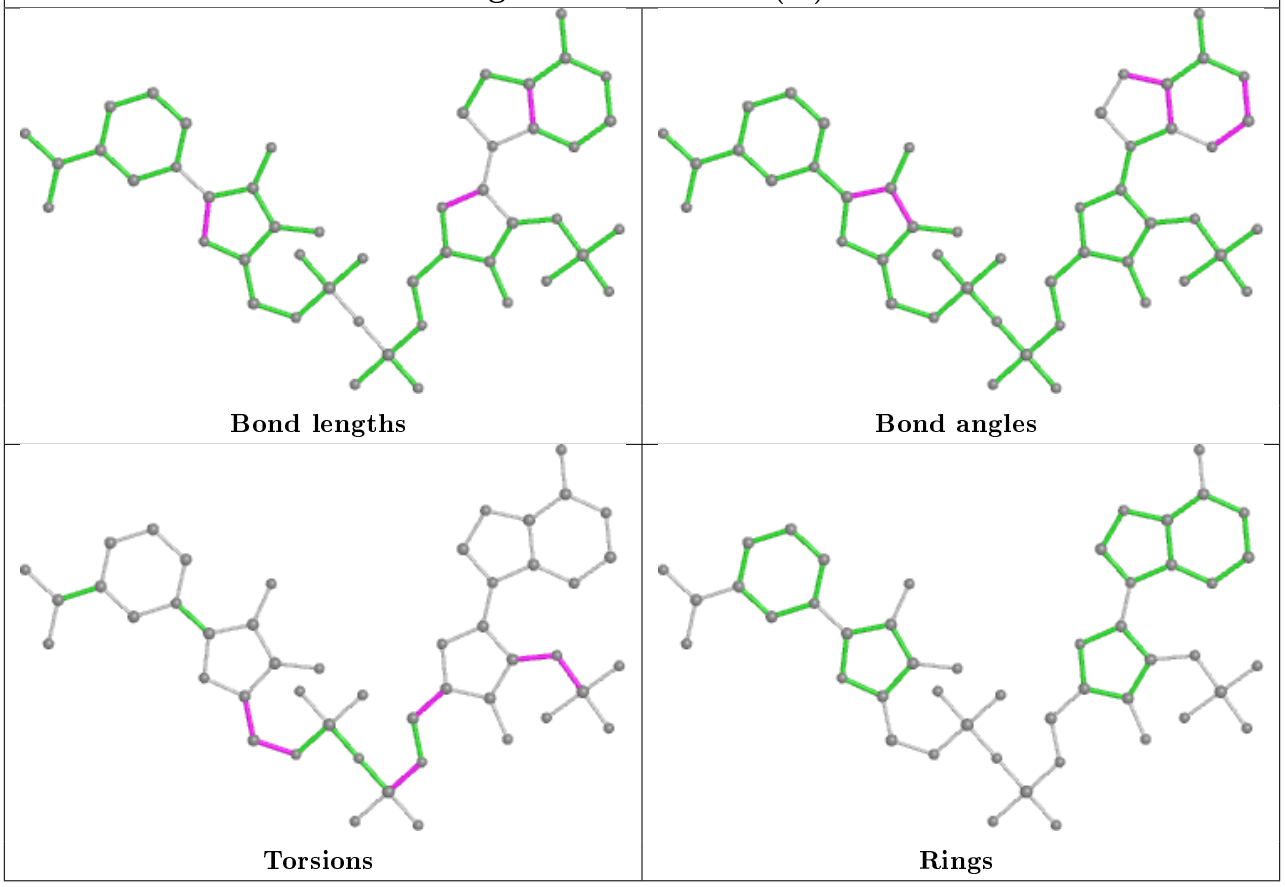


Torsions



Rings

Ligand NAP D 402 (A)



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	323/328 (98%)	0.18	8 (2%) 57 55	28, 47, 71, 96	0
1	B	323/328 (98%)	0.19	13 (4%) 38 33	27, 50, 86, 104	0
1	C	323/328 (98%)	0.01	4 (1%) 79 79	24, 39, 64, 100	0
1	D	323/328 (98%)	0.08	3 (0%) 84 84	24, 43, 74, 89	0
1	E	323/328 (98%)	0.05	10 (3%) 49 44	23, 40, 71, 112	0
1	F	323/328 (98%)	0.10	6 (1%) 66 65	24, 45, 76, 93	0
1	G	265/328 (80%)	2.52	132 (49%) 0 0	76, 113, 142, 171	0
1	H	323/328 (98%)	2.39	152 (47%) 0 0	71, 112, 154, 180	0
All	All	2526/2624 (96%)	0.65	328 (12%) 3 2	23, 50, 135, 180	0

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	91	VAL	11.6
1	H	42	TYR	11.1
1	H	291	GLY	10.9
1	H	300	ASN	10.4
1	H	288	TYR	9.0
1	G	63	PRO	8.8
1	G	225	GLU	8.8
1	H	189	GLY	8.4
1	H	71	PRO	8.4
1	G	100	VAL	8.2
1	H	282	THR	8.0
1	H	1	MET	8.0
1	G	64	PHE	7.7
1	G	71	PRO	7.5
1	G	1	MET	7.4
1	H	29	THR	7.4

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Mol	Chain	Res	Type	RSRZ
1	H	186	TYR	7.3
1	G	236	SER	7.2
1	G	134	LEU	7.2
1	G	289	ILE	7.1
1	H	304	ILE	7.1
1	H	120	PHE	7.1
1	H	270	GLY	6.9
1	H	274	MET	6.9
1	G	27	ILE	6.7
1	G	139	ALA	6.7
1	G	101	LYS	6.5
1	H	63	PRO	6.5
1	H	295	ALA	6.4
1	H	299	ALA	6.4
1	G	51	PHE	6.4
1	H	39	GLU	6.3
1	E	300	ASN	6.3
1	G	19	ALA	6.1
1	G	133	THR	6.0
1	G	227	THR	5.9
1	H	239	ILE	5.9
1	G	95	GLU	5.9
1	G	148	PHE	5.9
1	G	220	VAL	5.9
1	H	99	THR	5.9
1	H	116	TYR	5.8
1	G	267	ASN	5.8
1	H	97	VAL	5.8
1	H	30	LEU	5.8
1	H	175	LEU	5.6
1	G	231	GLU	5.6
1	H	94	PHE	5.6
1	H	119	ARG	5.5
1	G	221	THR	5.5
1	G	223	ILE	5.5
1	H	5	GLU	5.5
1	G	107	PHE	5.4
1	H	122	THR	5.4
1	G	117	GLU	5.3
1	G	303	PHE	5.3
1	H	41	ILE	5.3
1	G	136	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
1	H	121	LEU	5.3
1	G	26	GLY	5.2
1	G	224	THR	5.2
1	G	140	ASP	5.2
1	H	268	GLU	5.2
1	G	13	PRO	5.2
1	D	296	GLY	5.1
1	H	238	THR	4.9
1	G	113	LYS	4.9
1	H	180	ALA	4.9
1	G	11	GLY	4.8
1	H	216	PHE	4.8
1	H	308	LYS	4.8
1	H	38	VAL	4.8
1	G	244	VAL	4.7
1	H	70	LYS	4.7
1	G	309	PHE	4.7
1	H	281	GLU	4.7
1	G	57	LEU	4.7
1	G	297	ASN	4.7
1	G	301	THR	4.6
1	H	114	ASP	4.6
1	H	127	TYR	4.6
1	H	31	ILE	4.6
1	G	115	VAL	4.5
1	H	61	ASP	4.5
1	G	129	GLY	4.5
1	G	105	ASN	4.5
1	H	285	GLU	4.5
1	H	98	LEU	4.5
1	H	21	GLU	4.4
1	E	323	GLN	4.4
1	G	92	ASN	4.4
1	B	323	GLN	4.4
1	G	156	ASP	4.4
1	G	147	TYR	4.3
1	G	228	VAL	4.3
1	C	268	GLU	4.3
1	G	18	ALA	4.3
1	G	154	TYR	4.3
1	G	141	LEU	4.2
1	H	108	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	H	129	GLY	4.2
1	H	110	THR	4.2
1	H	233	ASN	4.2
1	H	130	GLN	4.2
1	H	131	HIS	4.1
1	H	89	LEU	4.1
1	H	22	GLN	4.1
1	H	318	MET	4.1
1	G	265	ASN	4.1
1	G	251	HIS	4.1
1	B	300	ASN	4.0
1	H	2	GLN	4.0
1	G	114	ASP	4.0
1	G	3	LYS	4.0
1	H	203	PHE	4.0
1	H	7	ILE	3.9
1	H	160	VAL	3.9
1	G	29	THR	3.9
1	H	182	VAL	3.9
1	A	323	GLN	3.9
1	G	266	THR	3.9
1	G	290	ALA	3.9
1	G	118	CYS	3.9
1	H	100	VAL	3.9
1	H	128	TYR	3.8
1	G	2	GLN	3.8
1	H	3	LYS	3.8
1	G	226	ASP	3.8
1	H	218	ALA	3.8
1	H	271	THR	3.8
1	H	289	ILE	3.8
1	H	185	LEU	3.8
1	G	69	SER	3.8
1	H	178	ALA	3.8
1	H	260	VAL	3.8
1	H	294	ALA	3.8
1	H	151	ALA	3.7
1	H	272	ALA	3.7
1	G	120	PHE	3.7
1	G	264	ILE	3.7
1	G	234	GLY	3.6
1	G	132	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	298	ASP	3.6
1	H	118	CYS	3.6
1	G	261	GLY	3.6
1	H	26	GLY	3.6
1	G	25	LYS	3.6
1	G	288	TYR	3.6
1	H	224	THR	3.6
1	G	233	ASN	3.6
1	H	172	ALA	3.5
1	B	299	ALA	3.5
1	G	97	VAL	3.5
1	A	105	ASN	3.5
1	H	223	ILE	3.5
1	G	317	SER	3.5
1	H	188	GLY	3.4
1	D	297	ASN	3.4
1	H	319	LEU	3.4
1	G	138	GLY	3.4
1	H	275	TYR	3.4
1	G	157	GLN	3.4
1	G	230	TYR	3.4
1	H	68	GLU	3.3
1	H	109	ILE	3.3
1	H	264	ILE	3.3
1	G	10	GLY	3.3
1	G	318	MET	3.3
1	G	96	GLU	3.3
1	H	8	ILE	3.2
1	A	300	ASN	3.2
1	H	69	SER	3.2
1	G	47	HIS	3.2
1	H	105	ASN	3.2
1	G	143	LYS	3.2
1	G	65	ILE	3.2
1	G	280	TYR	3.2
1	G	5	GLU	3.2
1	G	135	GLU	3.2
1	H	320	ALA	3.1
1	G	222	GLN	3.1
1	G	269	PHE	3.1
1	H	254	TYR	3.1
1	G	300	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	298	ASP	3.1
1	H	142	PRO	3.1
1	H	181	ASN	3.1
1	H	302	ILE	3.1
1	H	78	VAL	3.1
1	H	90	LYS	3.1
1	G	119	ARG	3.0
1	H	4	VAL	3.0
1	H	19	ALA	3.0
1	B	1	MET	3.0
1	G	61	ASP	3.0
1	H	213	ASP	3.0
1	G	315	ALA	3.0
1	H	123	ILE	3.0
1	H	62	VAL	3.0
1	G	302	ILE	3.0
1	E	1	MET	3.0
1	G	56	LYS	2.9
1	H	27	ILE	2.9
1	G	294	ALA	2.9
1	H	103	MET	2.9
1	F	1	MET	2.9
1	G	235	GLU	2.9
1	G	87	HIS	2.9
1	H	53	SER	2.9
1	G	34	LYS	2.9
1	H	24	ARG	2.9
1	H	20	ILE	2.8
1	H	170	ASP	2.8
1	B	105	ASN	2.8
1	H	267	ASN	2.8
1	G	22	GLN	2.8
1	H	32	ILE	2.8
1	H	115	VAL	2.8
1	H	88	GLN	2.8
1	G	239	ILE	2.8
1	E	269	PHE	2.8
1	H	132	ASN	2.8
1	G	152	HIS	2.8
1	G	254	TYR	2.7
1	G	158	ASP	2.7
1	G	20	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	294	ALA	2.7
1	G	252	PRO	2.7
1	G	103	MET	2.7
1	G	238	THR	2.7
1	H	35	GLY	2.7
1	G	310	HIS	2.7
1	G	146	HIS	2.7
1	A	118	CYS	2.6
1	H	125	THR	2.6
1	G	24	ARG	2.6
1	G	316	GLN	2.6
1	G	229	THR	2.6
1	H	179	GLY	2.6
1	H	133	THR	2.6
1	H	16	LEU	2.6
1	G	151	ALA	2.6
1	H	199	ILE	2.6
1	C	266	THR	2.6
1	G	268	GLU	2.6
1	E	117	GLU	2.5
1	H	104	ASN	2.5
1	G	155	PHE	2.5
1	H	298	ASP	2.5
1	F	267	ASN	2.5
1	H	276	ASN	2.5
1	B	276	ASN	2.4
1	G	260	VAL	2.4
1	H	126	GLY	2.4
1	H	321	LYS	2.4
1	G	80	TYR	2.4
1	H	23	LYS	2.4
1	H	65	ILE	2.4
1	A	286	ASN	2.4
1	H	77	LEU	2.4
1	G	232	VAL	2.4
1	H	222	GLN	2.4
1	G	246	ALA	2.4
1	H	273	PRO	2.4
1	H	144	VAL	2.3
1	H	46	THR	2.3
1	H	257	LEU	2.3
1	G	299	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	243	TYR	2.3
1	H	111	THR	2.3
1	D	233	ASN	2.3
1	H	296	GLY	2.3
1	G	284	ILE	2.3
1	H	317	SER	2.3
1	E	30	LEU	2.3
1	G	99	THR	2.3
1	H	303	PHE	2.3
1	G	6	SER	2.3
1	E	268	GLU	2.3
1	G	245	PHE	2.3
1	H	52	SER	2.3
1	G	128	TYR	2.3
1	H	9	ILE	2.3
1	G	237	LYS	2.3
1	H	64	PHE	2.3
1	F	316	GLN	2.3
1	H	261	GLY	2.2
1	A	120	PHE	2.2
1	F	323	GLN	2.2
1	H	280	TYR	2.2
1	E	267	ASN	2.2
1	H	149	LYS	2.2
1	G	263	GLN	2.2
1	H	316	GLN	2.2
1	E	299	ALA	2.2
1	G	150	GLU	2.2
1	F	233	ASN	2.2
1	G	70	LYS	2.2
1	C	137	GLU	2.2
1	G	102	LYS	2.2
1	H	152	HIS	2.1
1	B	90	LYS	2.1
1	F	298	ASP	2.1
1	B	270	GLY	2.1
1	H	40	SER	2.1
1	H	107	PHE	2.1
1	G	149	LYS	2.1
1	H	251	HIS	2.1
1	H	221	THR	2.1
1	H	301	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	237	LYS	2.1
1	B	225	GLU	2.1
1	G	75	GLN	2.1
1	H	286	ASN	2.1
1	G	320	ALA	2.1
1	H	34	LYS	2.1
1	H	50	PHE	2.0
1	H	146	HIS	2.0
1	C	239	ILE	2.0
1	G	314	ILE	2.0
1	H	183	THR	2.0
1	A	19	ALA	2.0
1	B	120	PHE	2.0
1	G	287	CYS	2.0
1	H	173	LEU	2.0
1	H	85	LYS	2.0
1	E	32	ILE	2.0
1	B	269	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	H	401	53/53	0.69	0.44	92,114,133,136	0
3	NAP	F	402	48/48	0.78	0.40	53,68,85,96	0
3	NAP	D	402[B]	48/48	0.79	0.43	40,55,65,67	48
3	NAP	D	402[A]	48/48	0.79	0.43	38,56,64,68	48
2	FAD	G	401	53/53	0.83	0.26	73,94,100,103	0

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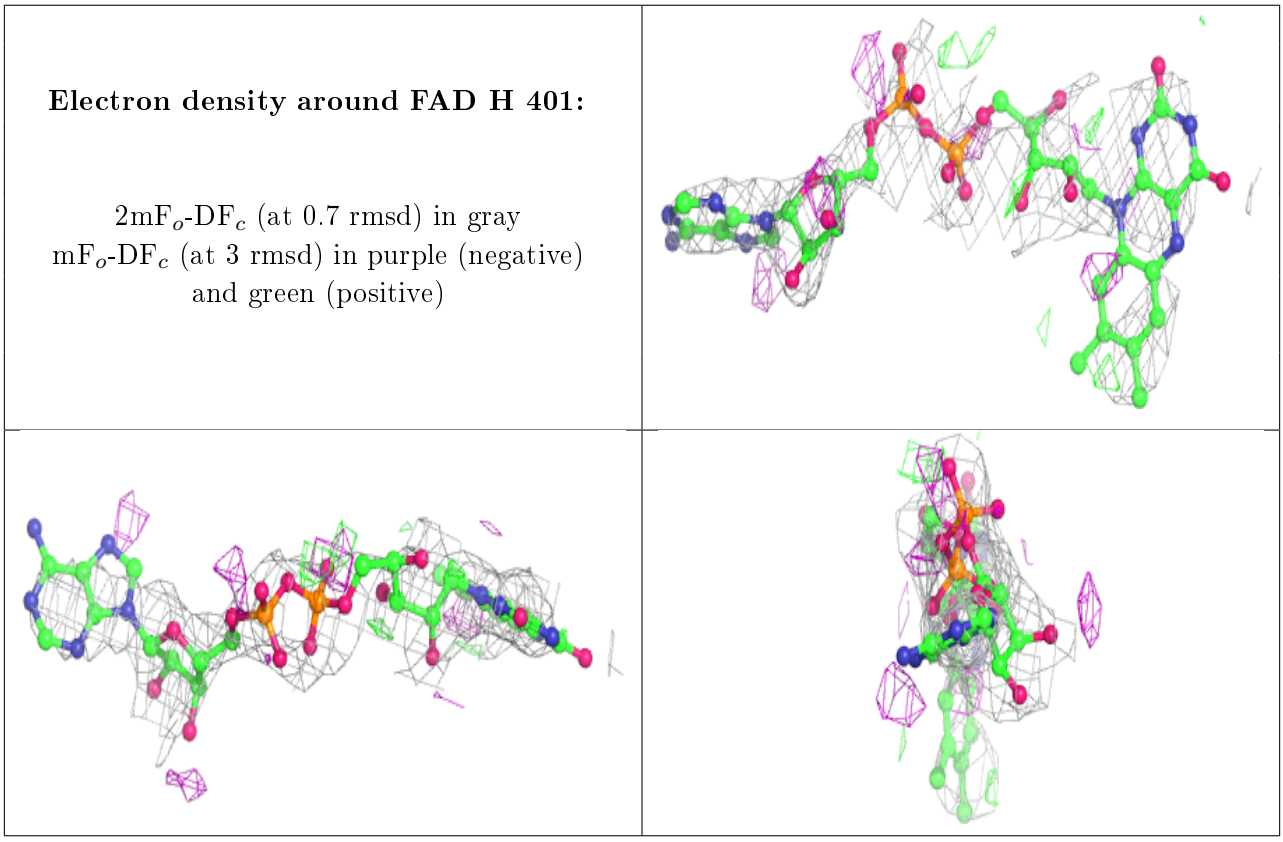
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAP	C	402	48/48	0.87	0.29	41,53,62,70	0
2	FAD	A	401	53/53	0.96	0.16	29,39,45,47	0
2	FAD	B	401	53/53	0.96	0.19	37,44,54,64	0
2	FAD	D	401	53/53	0.97	0.18	28,35,41,46	0
2	FAD	F	401	53/53	0.97	0.18	32,39,44,49	0
2	FAD	C	401	53/53	0.98	0.17	24,35,40,43	0
2	FAD	E	401	53/53	0.98	0.15	24,33,39,42	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.

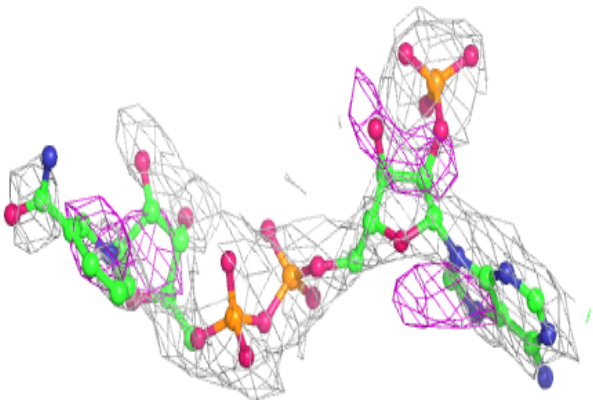
Electron density around FAD H 401:

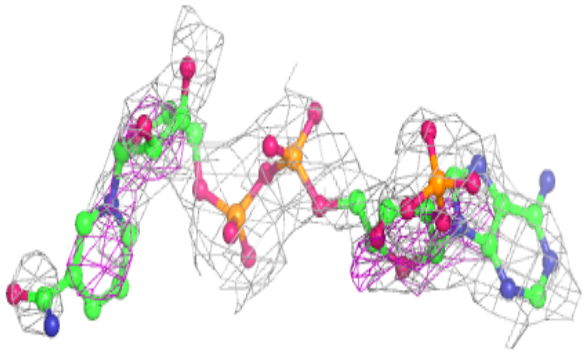
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

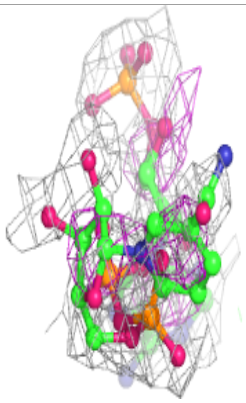


Electron density around NAP F 402:

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

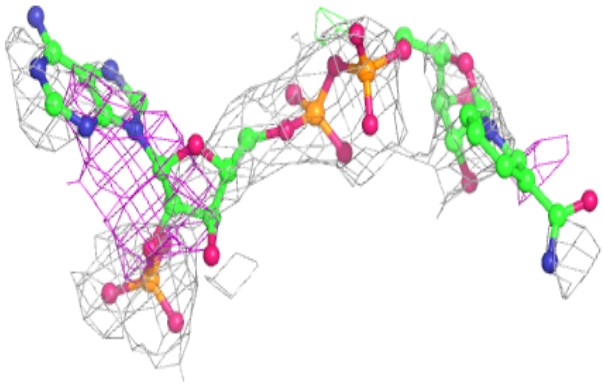


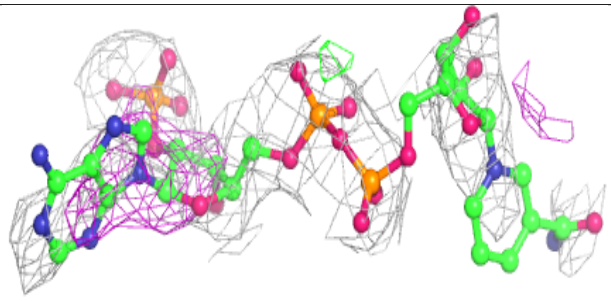


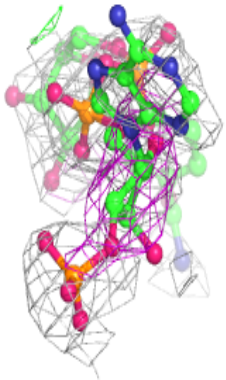


Electron density around NAP D 402 (B):

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

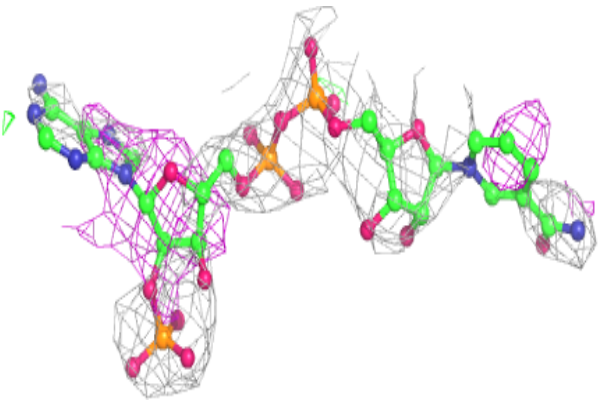


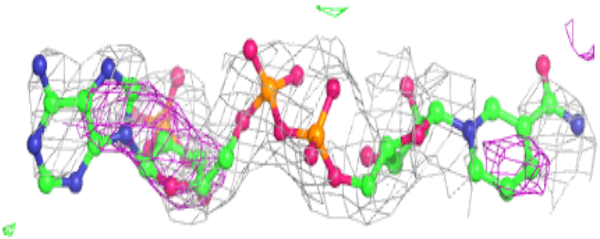


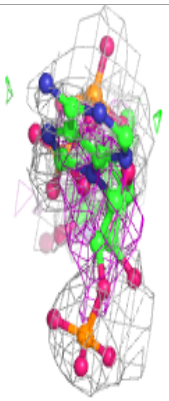


Electron density around NAP D 402 (A):

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

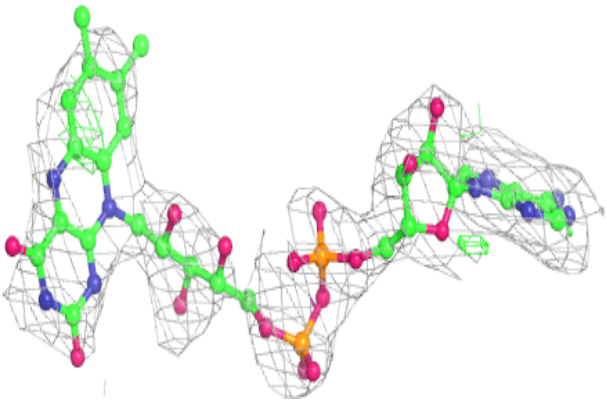


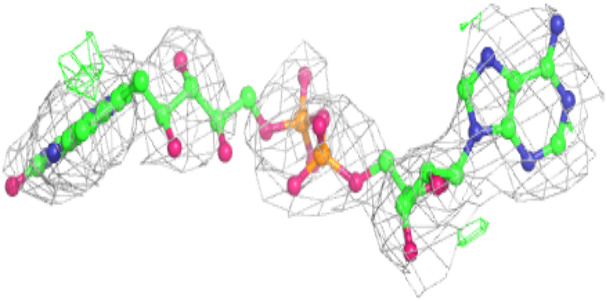


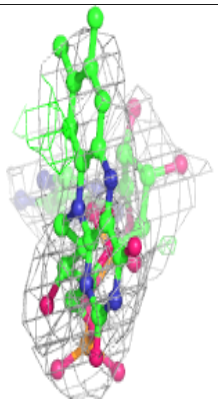


Electron density around FAD G 401:

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

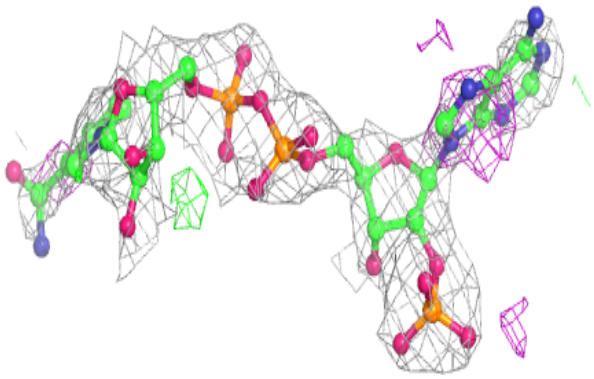


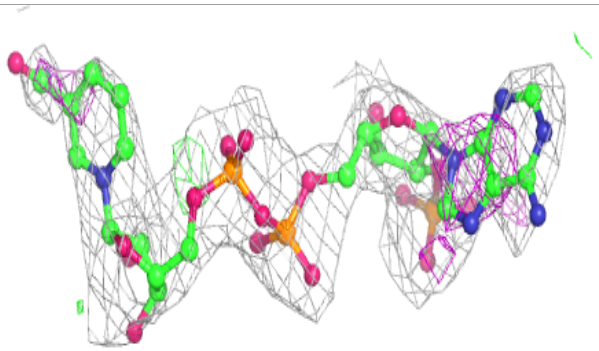


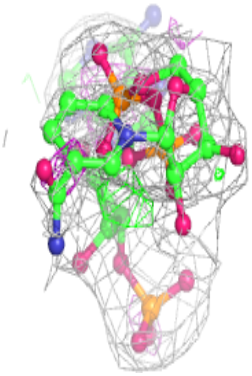


Electron density around NAP C 402:

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

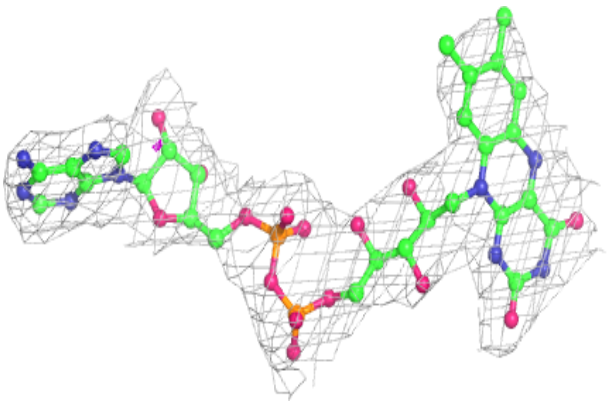


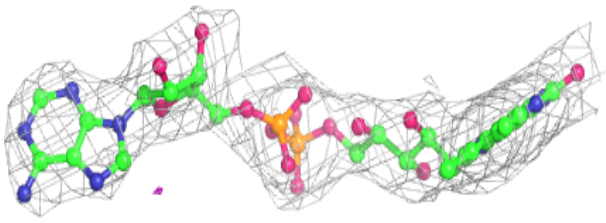


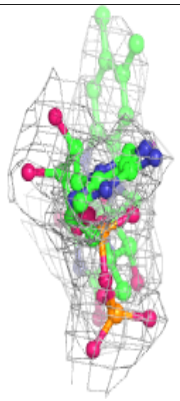


Electron density around FAD A 401:

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

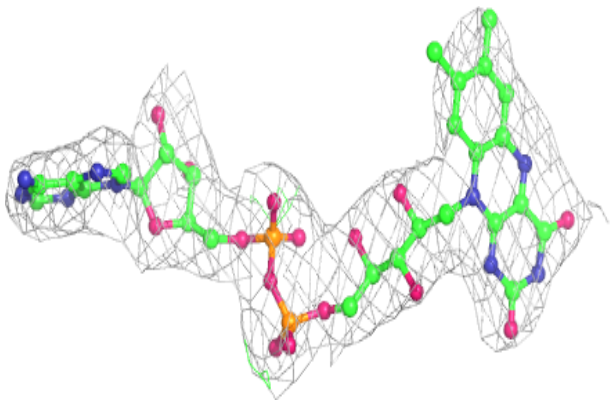


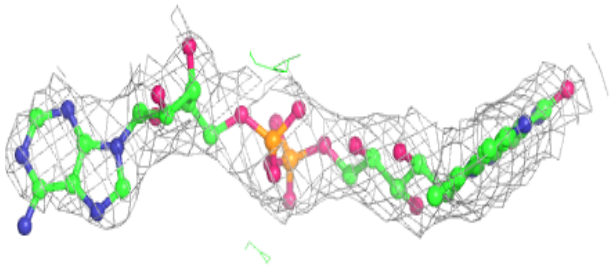


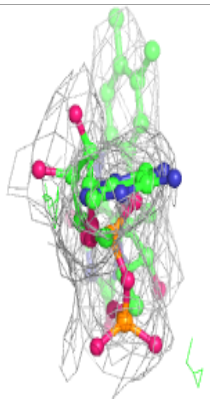


Electron density around FAD B 401:

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

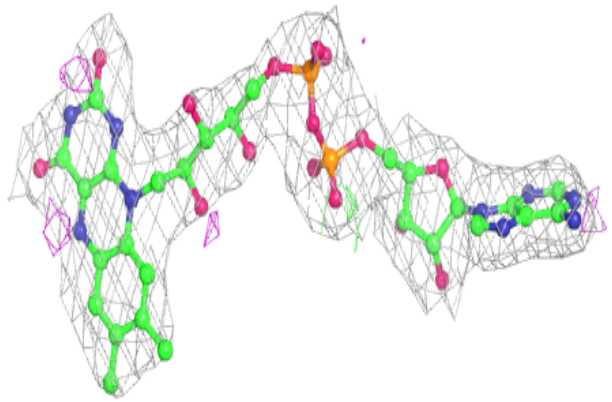


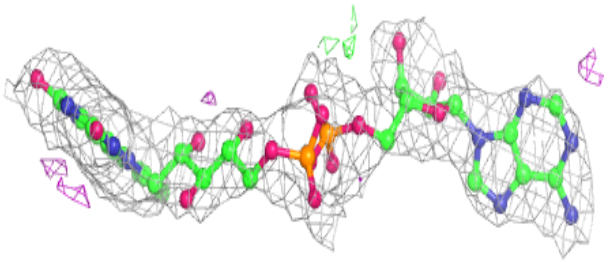


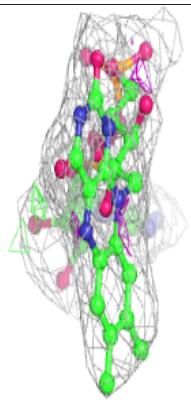


Electron density around FAD D 401:

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

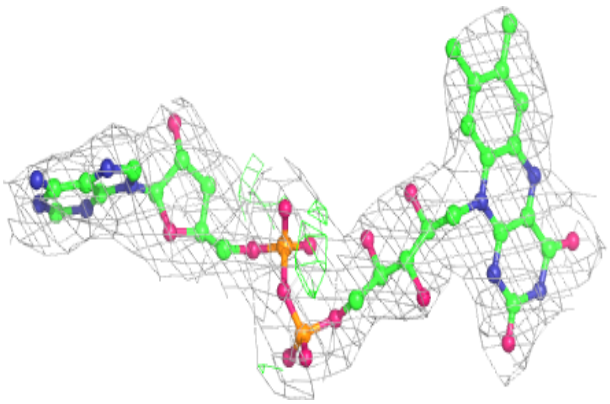


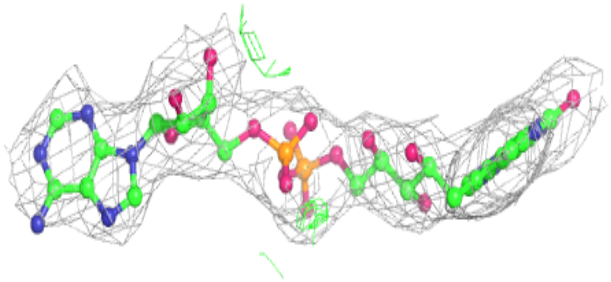


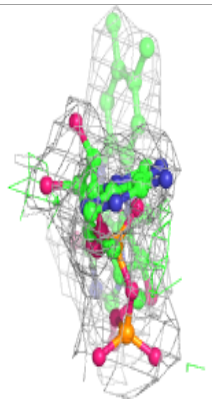


Electron density around FAD F 401:

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

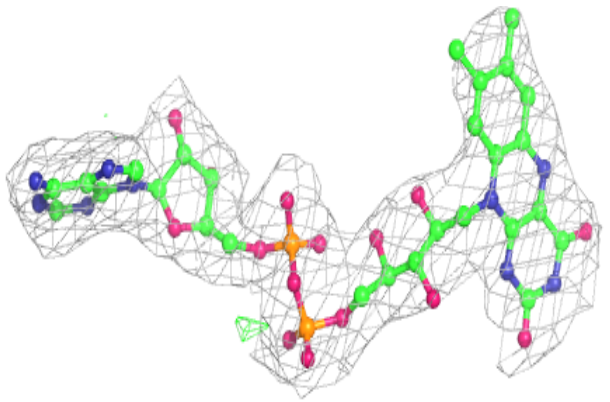


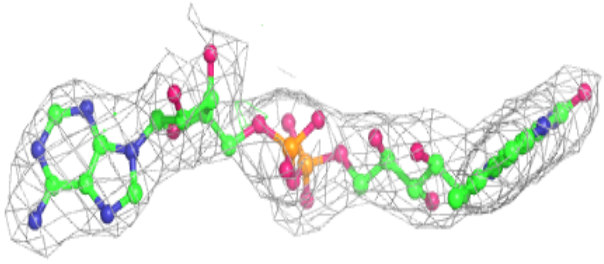


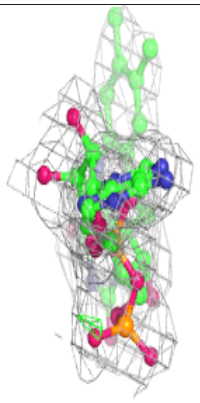


Electron density around FAD C 401:

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

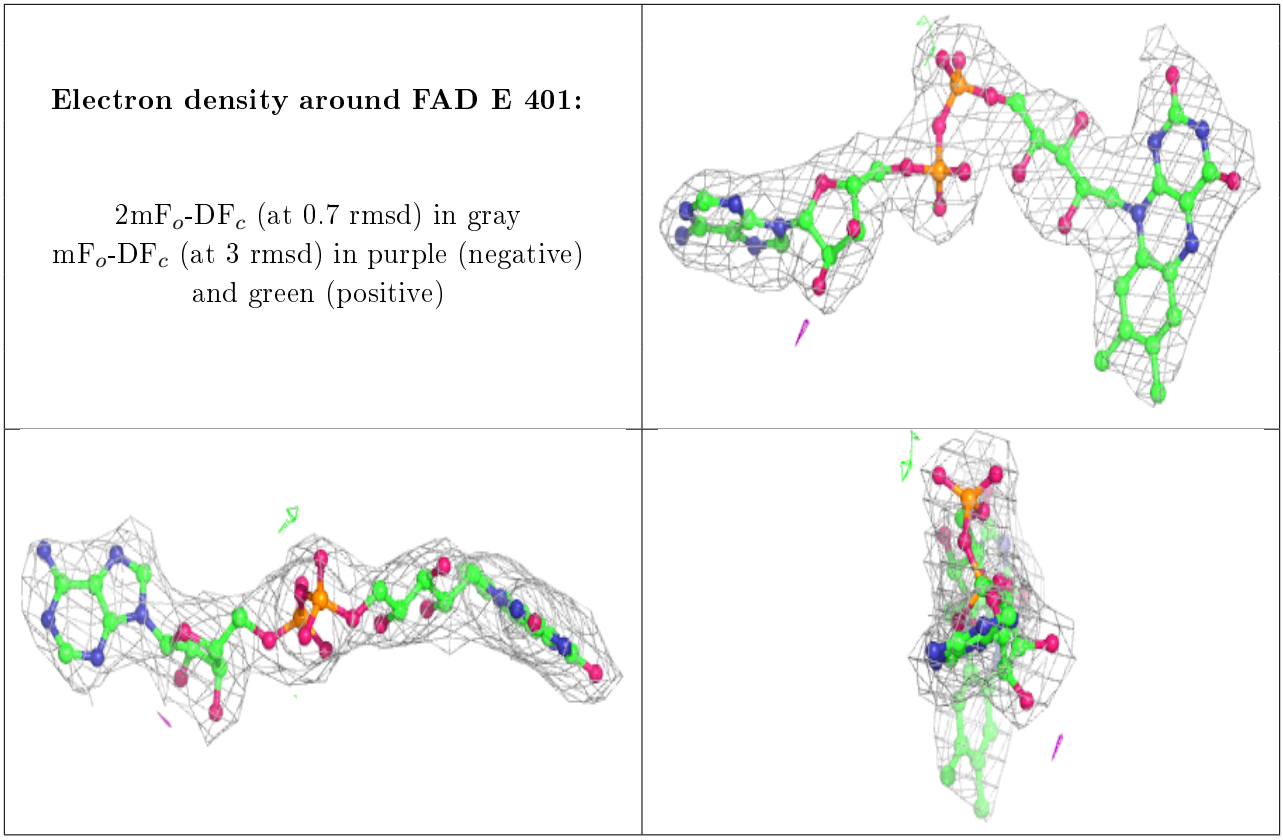






Electron density around FAD E 401:

$2mF_o$-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

There are no such residues in this entry.