



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:54 PM UTC

PDB ID : 7A7B / pdb_00007a7b
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 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

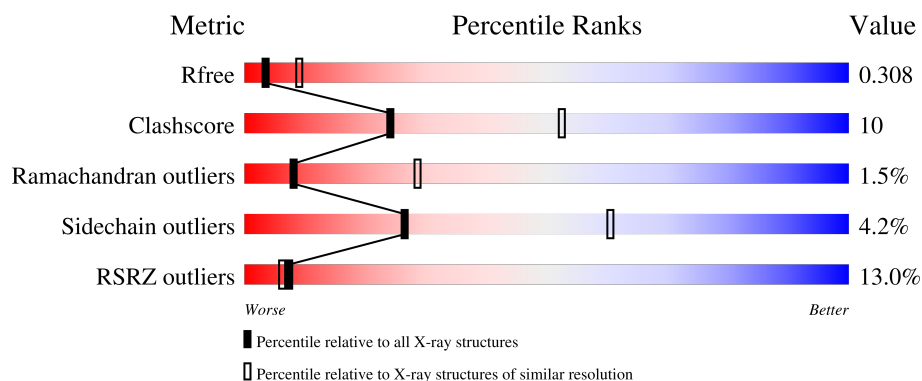
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. 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	328	2% 78% 19% ..
1	B	328	2% 82% 15% ..
1	C	328	% 76% 21% ..
1	D	328	% 74% 23% ..
1	E	328	% 80% 18% .

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

2 Entry composition

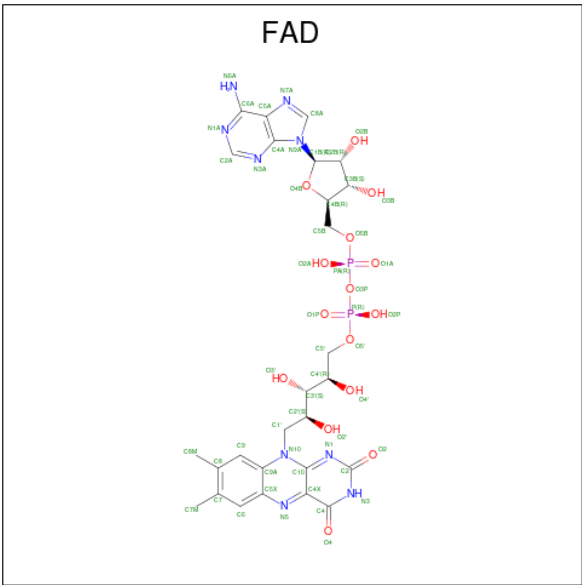
There are 4 unique types of molecules in this entry. The entry contains 20666 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

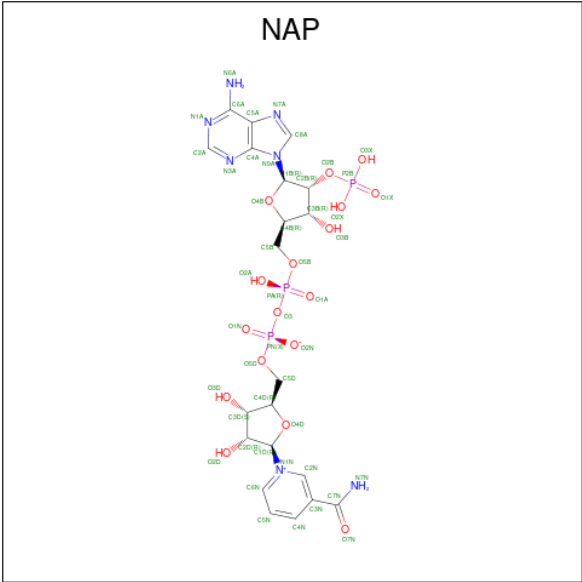
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2554	1633	420	492	9			
1	B	323	Total	C	N	O	S	0	0	0
			2554	1633	420	492	9			
1	C	323	Total	C	N	O	S	0	1	0
			2560	1637	421	493	9			
1	D	323	Total	C	N	O	S	0	1	0
			2565	1642	421	493	9			
1	E	323	Total	C	N	O	S	0	1	0
			2559	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 (CCD ID: 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 (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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		

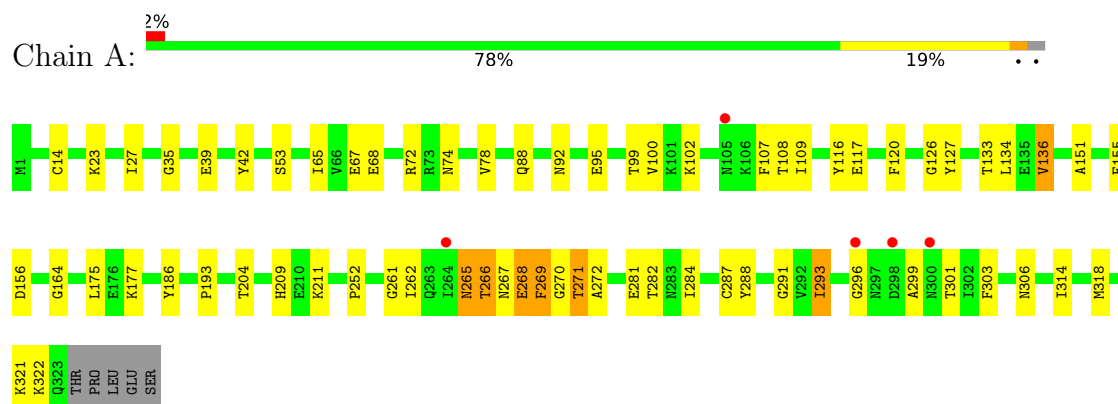
- Molecule 4 is water.

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		

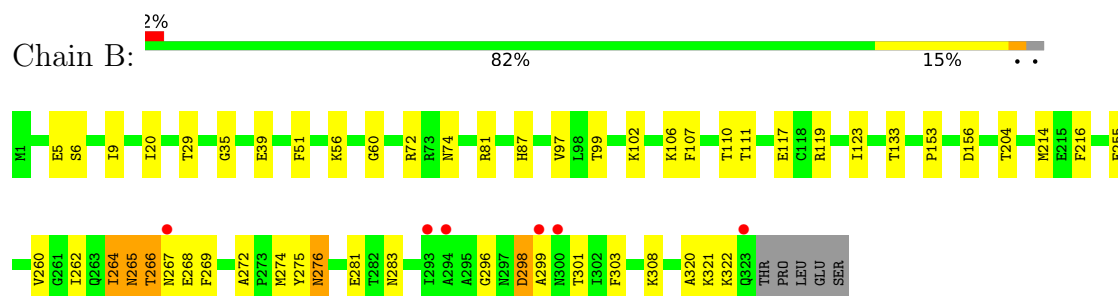
3 Residue-property plots

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.

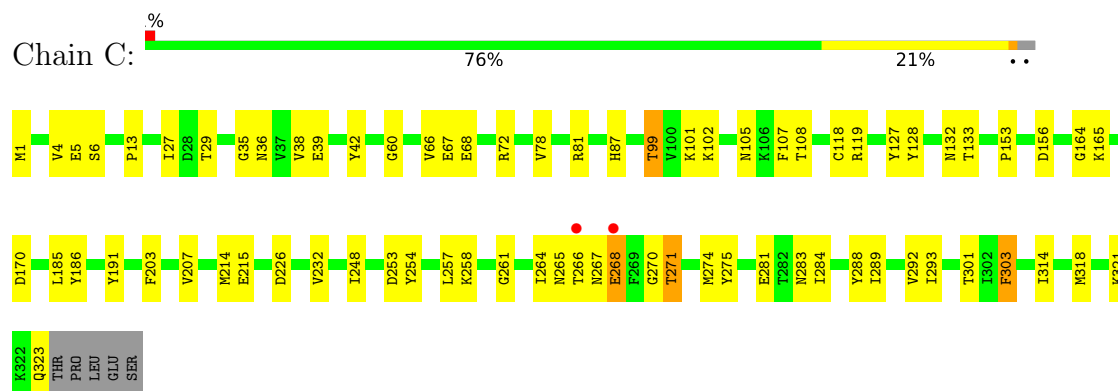
- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr



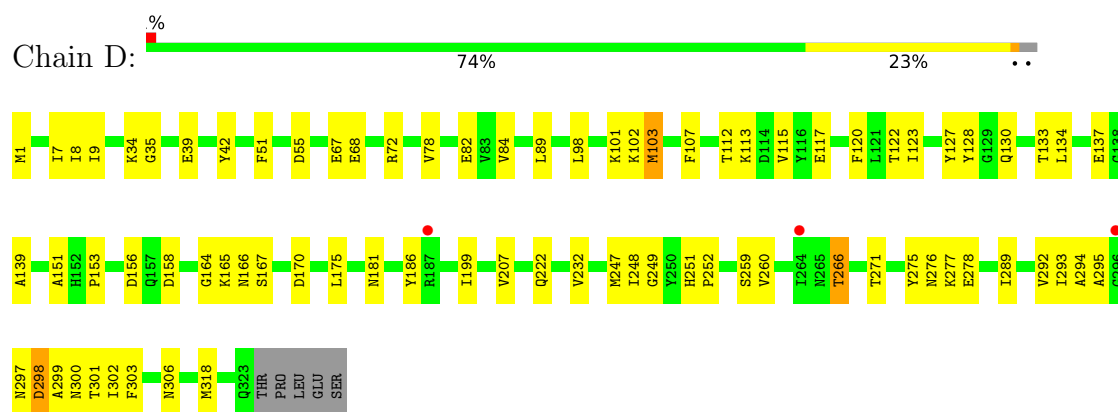
- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr



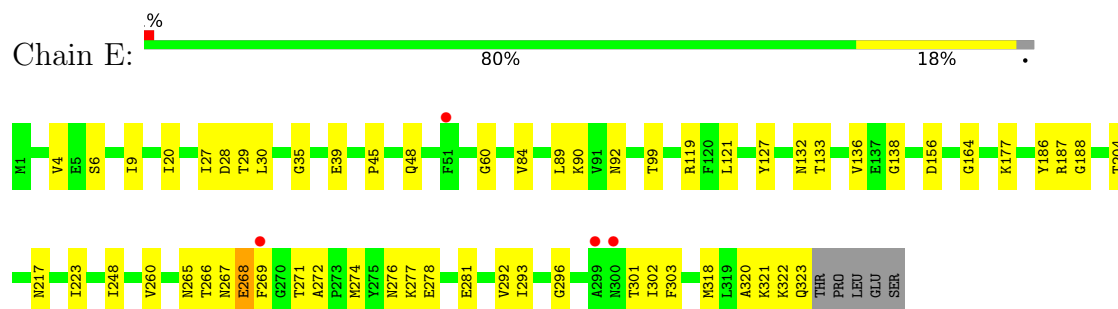
- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr



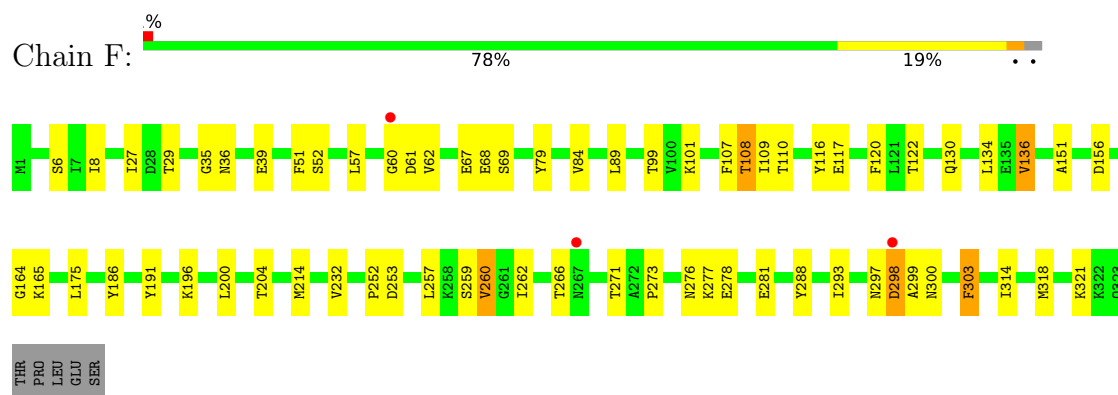
- Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr



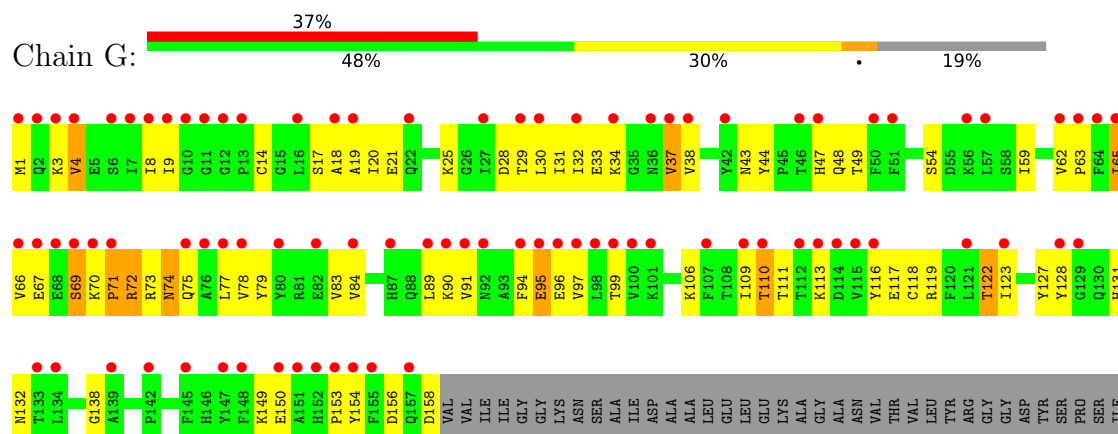
• Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr

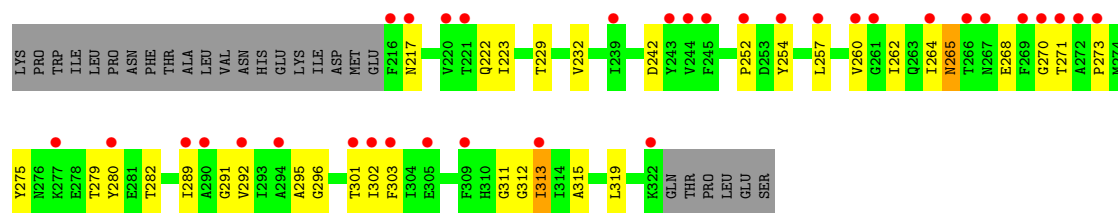


• Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr

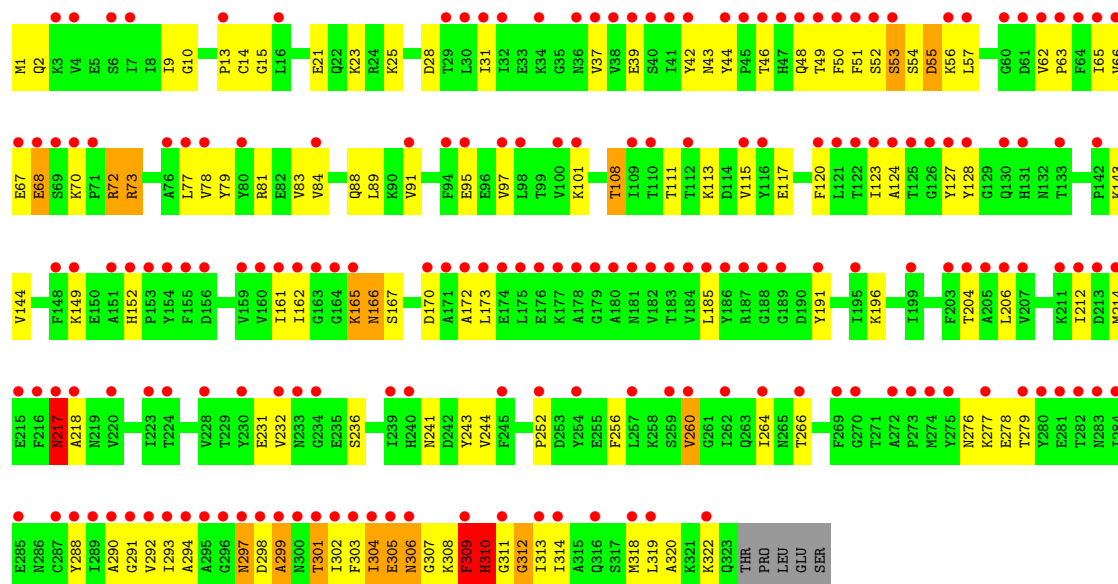


• Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr





● Molecule 1: YpdA family putative bacillithiol disulfide reductase Bdr



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 0.249 , 0.308	Depositor DCC
R_{free} test set	3683 reflections (4.98%)	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 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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.*

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: 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	0.43	0/2610	0.68	2/3537 (0.1%)
1	B	0.42	0/2610	0.64	0/3537
1	C	0.47	0/2619	0.71	1/3549 (0.0%)
1	D	0.44	0/2622	0.70	0/3553
1	E	0.47	0/2618	0.70	0/3548
1	F	0.44	0/2627	0.70	0/3560
1	G	0.32	0/2159	0.54	0/2921
1	H	0.37	0/2610	0.75	0/3537
All	All	0.42	0/20475	0.68	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(°)	Ideal(°)
1	C	268	GLU	N-CA-C	-5.67	106.17	112.57
1	A	53	SER	CA-C-N	-5.18	112.55	121.66
1	A	53	SER	C-N-CA	-5.18	112.55	121.66

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

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	49	0
1	B	2554	0	2506	31	0
1	C	2560	0	2514	48	0
1	D	2565	0	2514	58	0
1	E	2559	0	2512	31	0
1	F	2565	0	2516	47	0
1	G	2113	0	2058	75	0
1	H	2554	0	2506	88	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	2	0
2	E	53	0	31	0	0
2	F	53	0	31	1	0
2	G	53	0	31	4	0
2	H	53	0	31	5	0
3	C	48	0	25	4	0
3	D	96	0	50	17	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	405	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 10.

All (405) 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:F:27:ILE:HD13	1:F:318:MET:HE2	1.58	0.84
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:D:120:PHE:HB3	1:D:318:MET:HE2	1.64	0.80
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:27:ILE:HD13	1:A:318:MET:HE2	1.80	0.62
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:G:70:LYS:C	1:G:72:ARG:H	2.07	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:B:56:LYS:O	1:B:308:LYS:NZ	2.32	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:H:120:PHE:HB3	1:H:318:MET:HE2	1.83	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:E:27:ILE:HD13	1:E:318:MET:HE2	1.84	0.59
1:G:49:THR:HA	1:G:72:ARG:HA	1.83	0.59
1:C:27:ILE:HD13	1:C:318:MET:HE2	1.85	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: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:A:261:GLY:C	1:A:284:ILE:HD11	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:165:LYS:HD2	3:D:402[B]:NAP:H51A	1.85	0.57
1:F:62:VAL:O	1:F:79:TYR:OH	2.19	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
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:F:191:TYR:CE1	1:F:214:MET:HE2	2.41	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: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:O	1:H:54:SER:OG	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:D:98:LEU:HD11	1:D:112:THR:HG22	1.88	0.55
1:H:65:ILE:HG12	1:H:66:VAL:H	1.71	0.55
1:H:101:LYS:HB2	1:H:108:THR:HG23	1.89	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:E:281:GLU:OE2	1:E:321:LYS:NZ	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:402:NAP:O5D	3:C:402:NAP:H6N	2.08	0.53
1:B:102:LYS:HD2	1:B:106:LYS:O	2.08	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:C:68:GLU:CD	1:C:72:ARG:HH22	2.17	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:B:276:ASN:HD22	1:B:276:ASN:C	2.15	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:E:267:ASN:CG	1:E:268:GLU:H	2.18	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:C:281:GLU:CD	1:C:321:LYS:HZ1	2.19	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: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:51[A]:PHE:CE1	1:D:199:ILE:HD11	2.47	0.50
1:D:127:TYR:HE1	1:D:128:TYR:CZ	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:137:GLU:CD	1:D:222:GLN:HE21	2.20	0.50
1:H:21:GLU:HG3	1:H:310:HIS:CB	2.35	0.50
1:G:33:GLU:OE2	2:G:401:FAD:O3B	2.28	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:67:GLU:HA	1:D:78:VAL:HG21	1.94	0.49
1:A:266:THR:HB	1:A:271:THR:HG22	1.95	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: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:A:269:PHE:H	1:F:297:ASN:ND2	2.11	0.49
1:F:101:LYS:NZ	1:F:259:SER:O	2.42	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:95:GLU:OE2	1:A:116:TYR:OH	2.18	0.49
1:A:252:PRO:HB3	1:A:293:ILE:CD1	2.43	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:68:GLU:OE1	1:D:72:ARG:NH2	2.27	0.48
1:D:107:PHE:O	1:D:117:GLU:HA	2.13	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: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:E:177:LYS:HE2	1:F:67:GLU:O	2.13	0.48
1:F:51:PHE:CD2	3:F:402:NAP:H2N	2.49	0.48
1:F:52:SER:HB2	1:F:57:LEU:HD21	1.96	0.48
1:H:291:GLY:C	1:H:304:ILE:HD11	2.38	0.48
1:A:42:TYR:CE1	1:B:153:PRO:HD3	2.49	0.48
1:A:120:PHE:CB	1:A:318:MET:HE3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:261:GLY:CA	1:A:284:ILE:HD11	2.43	0.48
1:A:268:GLU:O	1:A:269:PHE:HB2	2.14	0.48
1:D:167:SER:H	3:D:402[A]:NAP:H51N	1.78	0.48
1:A:193:PRO:HG3	1:F:300:ASN:HD22	1.79	0.48
1:B:51:PHE:HZ	1:B:303:PHE:CD1	2.31	0.48
1:G:69:SER:OG	1:G:70:LYS:N	2.47	0.48
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:4:VAL:HG21	1:G:30:LEU:HD22	1.96	0.47
1:G:275:TYR:CE2	1:G:289:ILE:HD11	2.48	0.47
1:H:218:ALA:CB	1:H:232:VAL:HG22	2.43	0.47
1:C:226:ASP:N	1:C:226:ASP:OD1	2.47	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:A:164:GLY:HA3	1:A:186:TYR:CD1	2.49	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:G:99:THR:HB	1:G:110:THR:HB	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: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:A:120:PHE:CG	1:A:318:MET:HE3	2.50	0.46
1:B:268:GLU:HB3	1:B:269:PHE:H	1.48	0.46
2:C:401:FAD:O2'	2:C:401:FAD:O4'	2.26	0.46
1:G:43:ASN:HB2	1:G:128:TYR:HE2	1.80	0.46
1:H:49:THR:HG22	1:H:49:THR:O	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:F:298:ASP:C	1:F:300:ASN:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:120:PHE:CD2	1:F:318:MET:HE3	2.52	0.45
1:G:59:ILE:HG13	1:G:83:VAL:HG11	1.97	0.45
1:G:313:ILE:HD13	1:G:313:ILE:HA	1.79	0.45
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:C:191:TYR:CE1	1:C:214:MET:HE2	2.51	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:G:70:LYS:C	1:G:72:ARG:N	2.74	0.45
1:C:164:GLY:HA3	1:C:186:TYR:CE1	2.53	0.44
1:B:214:MET:HE3	1:B:216:PHE:CE1	2.52	0.44
1:C:165:LYS:HD3	3:C:402:NAP:O1A	2.17	0.44
1:C:253:ASP:O	1:C:257:LEU:HD12	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:H:1:MET:HE2	1:H:115:VAL:HG12	1.99	0.44
1:A:269:PHE:H	1:F:297:ASN:HD21	1.65	0.44
1:F:196:LYS:HA	1:F:196:LYS:HD3	1.81	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
1:H:72:ARG:HE	1:H:73:ARG:CZ	2.31	0.44
1:D:275:TYR:CZ	1:D:294:ALA:HB1	2.53	0.44
1:E:265:ASN:OD1	1:E:274:MET:HE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ASN:O	1:D:278:GLU:N	2.51	0.44
1:H:1:MET:HG2	1:H:2:GLN:N	2.31	0.44
1:H:144:VAL:HG22	1:H:244:VAL:HB	2.00	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:D:55:ASP:OD1	1:D:55:ASP:N	2.50	0.43
1:E:30:LEU:HD11	1:E:92:ASN:CG	2.43	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:H:97:VAL:HG22	1:H:111:THR:HG22	2.00	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
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:H9	2:H:401:FAD:H1'1	1.87	0.43
1:G:150:GLU:OE1	1:H:72:ARG:NH1	2.52	0.43
1:H:43:ASN:HB2	1:H:128:TYR:HH	1.81	0.43
1:H:124:ALA:HA	1:H:290:ALA:O	2.18	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:G:34:LYS:HE3	1:G:96:GLU:CD	2.43	0.43
1:H:84:VAL:HG13	1:H:89:LEU:HB2	2.01	0.43
1:A:74:ASN:O	1:A:78:VAL:HG23	2.19	0.42
1:A:151:ALA:HB1	1:A:175:LEU:HA	2.01	0.42
1:E:187:ARG:O	1:E:217:ASN:HA	2.19	0.42
1:H:55:ASP:C	1:H:57:LEU:H	2.27	0.42
1:H:294:ALA:HB3	1:H:302:ILE:HG21	2.01	0.42
1:A:127:TYR:CD1	1:A:127:TYR:C	2.97	0.42
1:D:113:LYS:HE2	1:D:113:LYS:HB3	1.85	0.42
1:H:66:VAL:HG23	1:H:67:GLU:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLY:HA3	1:A:186:TYR:CE1	2.55	0.42
1:B:255:GLU:H	1:B:255:GLU:CD	2.27	0.42
1:D:103:MET:HE2	1:D:103:MET:HB3	1.68	0.42
1:E:127:TYR:CD1	1:E:127:TYR:C	2.98	0.42
1:G:265:ASN:HB3	1:G:268:GLU:H	1.84	0.42
1:F:108:THR:O	1:F:108:THR:HG22	2.20	0.42
1:A:107:PHE:O	1:A:117:GLU:HA	2.20	0.42
1:A:322:LYS:HE3	1:A:322:LYS:HB2	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:HD2	1:G:149:LYS:HA	1.89	0.42
1:H:79:TYR:O	1:H:83:VAL:HG23	2.20	0.42
1:H:166:ASN:ND2	1:H:196:LYS:HG2	2.35	0.42
1:A:281:GLU:OE2	1:A:321:LYS:NZ	2.52	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
1:C:119:ARG:HH22	1:C:323:GLN:HB3	1.82	0.42
1:G:34:LYS:HB2	2:G:401:FAD:H1B	2.02	0.42
1:G:127:TYR:CE2	1:G:292:VAL:HB	2.55	0.42
1:H:288:TYR:CD2	1:H:314:ILE:HG23	2.55	0.42
1:A:100:VAL:HG13	1:A:109:ILE:HD13	2.01	0.42
1:A:102:LYS:HG2	1:A:107:PHE:CE1	2.54	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:B:281:GLU:CD	1:B:321:LYS:HZ1	2.28	0.41
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:O	1:H:217:ASN:ND2	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:O	1:B:276:ASN:ND2	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:F:109:ILE:HB	1:F:116:TYR:HB2	2.02	0.41
1:F:276:ASN:C	1:F:278:GLU:N	2.78	0.41
1:F:164:GLY:HA3	1:F:186:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:LEU:HD21	1:G:32:ILE:HD11	2.02	0.41
1:G:217:ASN:O	1:G:232:VAL:HA	2.20	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:H:191:TYR:CZ	1:H:214:MET:HE2	2.55	0.41
1:D:297:ASN:O	1:D:298:ASP:C	2.63	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:HG2	1:H:68:GLU:O	2.20	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:G:138:GLY:HA3	1:G:223:ILE:O	2.21	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
1:C:261:GLY:C	1:C:284:ILE:HD11	2.47	0.40
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
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:OD1	1:D:306:ASN:N	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:7:ILE:HD13	1:D:7:ILE:HG21	1.86	0.40
1:D:165:LYS:CD	3:D:402[B]:NAP:H3B	2.50	0.40
1:D:167:SER:HB3	1:D:247:MET:CE	2.51	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 ⓘ

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	321/328 (98%)	303 (94%)	17 (5%)	1 (0%)	36	65
1	B	321/328 (98%)	296 (92%)	22 (7%)	3 (1%)	14	41
1	C	322/328 (98%)	305 (95%)	16 (5%)	1 (0%)	36	65
1	D	322/328 (98%)	307 (95%)	11 (3%)	4 (1%)	10	34
1	E	322/328 (98%)	301 (94%)	20 (6%)	1 (0%)	36	65
1	F	323/328 (98%)	300 (93%)	18 (6%)	5 (2%)	8	28
1	G	261/328 (80%)	220 (84%)	34 (13%)	7 (3%)	4	16
1	H	321/328 (98%)	278 (87%)	27 (8%)	16 (5%)	1	6
All	All	2513/2624 (96%)	2310 (92%)	165 (7%)	38 (2%)	8	28

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

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Mol	Chain	Res	Type
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
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%)	265 (96%)	12 (4%)	26	60
1	B	277/282 (98%)	268 (97%)	9 (3%)	34	68
1	C	278/282 (99%)	271 (98%)	7 (2%)	42	74
1	D	278/282 (99%)	269 (97%)	9 (3%)	34	68
1	E	278/282 (99%)	266 (96%)	12 (4%)	26	60
1	F	279/282 (99%)	271 (97%)	8 (3%)	37	71
1	G	230/282 (82%)	213 (93%)	17 (7%)	13	38
1	H	277/282 (98%)	259 (94%)	18 (6%)	15	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2174/2256 (96%)	2082 (96%)	92 (4%)	26 60

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLU
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	293	ILE
1	B	133	THR
1	B	156	ASP
1	B	204	THR
1	B	260	VAL
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	99	THR
1	C	108	THR
1	C	133	THR
1	C	156	ASP
1	C	232	VAL
1	C	303	PHE
1	D	34	LYS
1	D	103	MET
1	D	133	THR
1	D	156	ASP
1	D	207	VAL
1	D	232	VAL
1	D	260	VAL
1	D	301	THR
1	D	303	PHE

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Mol	Chain	Res	Type
1	E	4	VAL
1	E	99	THR
1	E	133	THR
1	E	136	VAL
1	E	156	ASP
1	E	204	THR
1	E	260	VAL
1	E	266	THR
1	E	268	GLU
1	E	293	ILE
1	E	301	THR
1	E	303	PHE
1	F	108	THR
1	F	136	VAL
1	F	156	ASP
1	F	200	LEU
1	F	204	THR
1	F	232	VAL
1	F	260	VAL
1	F	303	PHE
1	G	4	VAL
1	G	29	THR
1	G	37	VAL
1	G	48	GLN
1	G	62	VAL
1	G	65	ILE
1	G	66	VAL
1	G	72	ARG
1	G	78	VAL
1	G	95	GLU
1	G	110	THR
1	G	122	THR
1	G	156	ASP
1	G	260	VAL
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	68	GLU

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Mol	Chain	Res	Type
1	H	73	ARG
1	H	108	THR
1	H	204	THR
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 (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	222	GLN
1	A	297	ASN
1	B	88	GLN
1	B	130	GLN
1	B	157	GLN
1	B	202	ASN
1	B	217	ASN
1	B	267	ASN
1	C	2	GLN
1	C	74	ASN
1	C	157	GLN
1	C	181	ASN
1	C	219	ASN
1	D	2	GLN
1	D	48	GLN
1	D	74	ASN
1	D	104	ASN
1	D	219	ASN
1	E	48	GLN
1	E	74	ASN
1	F	157	GLN
1	F	217	ASN
1	F	219	ASN
1	F	300	ASN

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Mol	Chain	Res	Type
1	G	75	GLN
1	H	43	ASN
1	H	276	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](#)

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
2	FAD	C	401	-	58,58,58	0.49	1 (1%)	85,89,89	0.55	2 (2%)
2	FAD	H	401	-	58,58,58	0.34	0	85,89,89	0.49	0
2	FAD	B	401	-	58,58,58	0.52	1 (1%)	85,89,89	0.71	2 (2%)
2	FAD	F	401	-	58,58,58	0.46	1 (1%)	85,89,89	0.49	1 (1%)
3	NAP	D	402[B]	-	50,52,52	1.27	6 (12%)	71,80,80	1.56	7 (9%)
3	NAP	F	402	-	50,52,52	1.52	6 (12%)	71,80,80	1.72	14 (19%)
2	FAD	D	401	-	58,58,58	0.48	0	85,89,89	0.42	0
2	FAD	G	401	-	58,58,58	0.41	0	85,89,89	0.43	1 (1%)
2	FAD	E	401	-	58,58,58	0.63	1 (1%)	85,89,89	0.57	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	C	402	-	50,52,52	1.46	7 (14%)	71,80,80	1.79	14 (19%)
2	FAD	A	401	-	58,58,58	0.49	1 (1%)	85,89,89	0.61	1 (1%)
3	NAP	D	402[A]	-	50,52,52	1.35	7 (14%)	71,80,80	1.57	10 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	401	-	-	0/34/50/50	0/6/6/6
2	FAD	H	401	-	-	8/34/50/50	0/6/6/6
2	FAD	B	401	-	-	4/34/50/50	0/6/6/6
2	FAD	F	401	-	-	3/34/50/50	0/6/6/6
3	NAP	D	402[B]	-	-	17/35/67/67	0/5/5/5
3	NAP	F	402	-	-	18/35/67/67	0/5/5/5
2	FAD	D	401	-	-	8/34/50/50	0/6/6/6
2	FAD	G	401	-	-	6/34/50/50	0/6/6/6
2	FAD	E	401	-	-	4/34/50/50	0/6/6/6
3	NAP	C	402	-	-	17/35/67/67	0/5/5/5
2	FAD	A	401	-	-	11/34/50/50	0/6/6/6
3	NAP	D	402[A]	-	-	13/35/67/67	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	NAP	C5A-C4A	5.98	1.49	1.39
3	F	402	NAP	C5A-C4A	5.69	1.49	1.39
3	D	402[A]	NAP	C5A-C4A	5.05	1.48	1.39
3	D	402[B]	NAP	C5A-C4A	5.02	1.48	1.39
3	D	402[A]	NAP	PA-O3	3.53	1.63	1.59
3	C	402	NAP	O4D-C1D	3.41	1.45	1.40
3	F	402	NAP	O4D-C1D	3.22	1.45	1.40
3	F	402	NAP	PN-O3	3.13	1.62	1.59
2	E	401	FAD	P-O3P	-3.12	1.56	1.59
3	D	402[B]	NAP	C5A-C6A	3.01	1.49	1.41
3	F	402	NAP	PA-O3	2.99	1.62	1.59
3	D	402[A]	NAP	C5A-C6A	2.98	1.49	1.41
3	C	402	NAP	C5A-C6A	2.97	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	402	NAP	C5A-C6A	2.94	1.49	1.41
3	C	402	NAP	C8A-N7A	2.80	1.37	1.31
2	B	401	FAD	P-O3P	-2.72	1.56	1.59
3	F	402	NAP	C8A-N7A	2.67	1.36	1.31
3	D	402[A]	NAP	PN-O3	2.66	1.62	1.59
3	D	402[A]	NAP	C8A-N7A	2.48	1.36	1.31
2	A	401	FAD	P-O2P	-2.47	1.43	1.55
3	D	402[B]	NAP	C8A-N7A	2.40	1.36	1.31
3	D	402[B]	NAP	PA-O3	2.36	1.62	1.59
3	D	402[A]	NAP	O4D-C1D	2.34	1.44	1.40
3	D	402[B]	NAP	PN-O3	2.32	1.62	1.59
2	C	401	FAD	P-O2P	-2.31	1.44	1.55
2	F	401	FAD	P-O2P	-2.22	1.45	1.55
3	C	402	NAP	PN-O3	2.21	1.61	1.59
3	C	402	NAP	P2B-O2B	2.18	1.63	1.59
3	D	402[B]	NAP	C5A-N7A	-2.15	1.35	1.39
3	C	402	NAP	C4A-N3A	2.06	1.38	1.34
3	D	402[A]	NAP	C5A-N7A	-2.01	1.35	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	NAP	C5A-C4A-N3A	-6.61	117.62	126.72
3	D	402[B]	NAP	C5A-C4A-N3A	-6.44	117.84	126.72
3	D	402[A]	NAP	C5A-C4A-N3A	-6.30	118.04	126.72
3	F	402	NAP	C5A-C4A-N3A	-6.03	118.42	126.72
3	C	402	NAP	N3A-C4A-N9A	5.77	136.97	127.17
3	D	402[B]	NAP	N3A-C4A-N9A	5.08	135.81	127.17
3	F	402	NAP	N3A-C4A-N9A	4.93	135.55	127.17
3	D	402[A]	NAP	N3A-C4A-N9A	4.80	135.33	127.17
2	B	401	FAD	C4'-C3'-C2'	-4.02	106.88	113.57
3	D	402[A]	NAP	C2A-N3A-C4A	3.94	121.45	111.83
3	D	402[B]	NAP	C2A-N3A-C4A	3.89	121.33	111.83
3	F	402	NAP	C2B-C1B-N9A	-3.75	107.59	113.75
3	D	402[B]	NAP	C4A-C5A-N7A	-3.70	106.35	110.58
3	C	402	NAP	C2A-N3A-C4A	3.67	120.81	111.83
3	D	402[A]	NAP	C4A-C5A-N7A	-3.64	106.42	110.58
3	F	402	NAP	C2A-N3A-C4A	3.56	120.54	111.83
3	D	402[A]	NAP	N3A-C2A-N1A	-3.32	123.56	128.58
3	D	402[B]	NAP	N3A-C2A-N1A	-3.16	123.80	128.58
3	C	402	NAP	C4A-C5A-N7A	-3.08	107.06	110.58
3	C	402	NAP	O3-PN-O1N	-3.06	101.51	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	NAP	N3A-C2A-N1A	-2.99	124.05	128.58
3	F	402	NAP	N3A-C2A-N1A	-2.99	124.06	128.58
2	A	401	FAD	O5'-P-O1P	-2.84	97.69	108.94
3	F	402	NAP	C4A-C5A-N7A	-2.83	107.34	110.58
3	D	402[B]	NAP	C5A-N7A-C8A	2.81	107.87	103.45
3	F	402	NAP	O3-PN-O1N	-2.79	102.32	110.70
3	C	402	NAP	O7N-C7N-C3N	-2.72	116.27	119.60
3	C	402	NAP	O3-PA-O1A	-2.70	102.57	110.70
3	C	402	NAP	C5A-N7A-C8A	2.67	107.64	103.45
3	D	402[A]	NAP	O2A-PA-O3	2.63	114.37	107.27
3	D	402[A]	NAP	C5A-N7A-C8A	2.59	107.52	103.45
3	D	402[A]	NAP	C4D-O4D-C1D	-2.55	107.59	109.92
3	F	402	NAP	C2B-C3B-C4B	2.51	107.38	101.99
3	F	402	NAP	C4D-O4D-C1D	2.50	112.21	109.92
3	C	402	NAP	C4A-N9A-C8A	2.48	108.35	105.74
3	C	402	NAP	C3N-C7N-N7N	2.42	120.71	117.74
2	B	401	FAD	C5'-C4'-C3'	2.37	116.69	112.22
3	D	402[B]	NAP	C4A-N9A-C8A	2.28	108.14	105.74
3	F	402	NAP	O2B-P2B-O1X	-2.26	101.28	109.33
3	C	402	NAP	C5N-C4N-C3N	-2.24	118.17	120.36
3	F	402	NAP	O5D-C5D-C4D	2.20	116.48	108.99
2	C	401	FAD	C4'-C3'-C2'	-2.19	109.92	113.57
3	C	402	NAP	O3X-P2B-O2X	2.14	115.84	107.80
3	F	402	NAP	C2D-C3D-C4D	2.12	106.70	102.61
2	E	401	FAD	C4'-C3'-C2'	-2.10	110.08	113.57
3	D	402[A]	NAP	C6A-C5A-N7A	2.08	136.11	132.09
2	G	401	FAD	C4'-C3'-C2'	-2.06	110.14	113.57
3	C	402	NAP	N6A-C6A-N1A	2.06	122.96	118.38
3	F	402	NAP	C2A-N1A-C6A	2.05	122.09	118.73
3	F	402	NAP	O3-PA-O1A	-2.04	104.56	110.70
2	F	401	FAD	O2A-PA-O3P	2.01	112.71	107.27
2	C	401	FAD	O2A-PA-O3P	2.01	112.71	107.27
3	D	402[A]	NAP	C2B-C3B-C4B	2.01	106.31	101.99

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FAD	C5B-O5B-PA-O2A
2	A	401	FAD	C5'-O5'-P-O1P
2	A	401	FAD	C5'-O5'-P-O2P
2	A	401	FAD	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
2	D	401	FAD	C5B-O5B-PA-O1A
2	D	401	FAD	C5B-O5B-PA-O2A
2	D	401	FAD	C5B-O5B-PA-O3P
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	C	402	NAP	C5B-O5B-PA-O2A
3	C	402	NAP	C5B-O5B-PA-O3
3	C	402	NAP	C2N-C3N-C7N-N7N
3	D	402[A]	NAP	C5B-O5B-PA-O2A
3	D	402[A]	NAP	C5B-O5B-PA-O3
3	D	402[A]	NAP	O4B-C4B-C5B-O5B
3	D	402[B]	NAP	C5B-O5B-PA-O1A
3	D	402[B]	NAP	C5B-O5B-PA-O2A
3	D	402[B]	NAP	C5B-O5B-PA-O3
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	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	F	402	NAP	C4N-C3N-C7N-O7N
3	C	402	NAP	C4N-C3N-C7N-N7N
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-O7N
3	C	402	NAP	C2N-C3N-C7N-O7N
2	H	401	FAD	C2'-C3'-C4'-O4'
3	F	402	NAP	O4B-C4B-C5B-O5B
3	F	402	NAP	C3B-C4B-C5B-O5B
2	H	401	FAD	C2'-C3'-C4'-C5'
2	H	401	FAD	O3'-C3'-C4'-O4'
2	A	401	FAD	O4B-C4B-C5B-O5B
3	D	402[A]	NAP	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	H	401	FAD	O3'-C3'-C4'-C5'
3	F	402	NAP	C1B-C2B-O2B-P2B
3	C	402	NAP	C3B-C2B-O2B-P2B
3	D	402[A]	NAP	C3B-C2B-O2B-P2B
3	F	402	NAP	C3B-C2B-O2B-P2B
2	D	401	FAD	C3B-C4B-C5B-O5B
3	D	402[A]	NAP	O4D-C4D-C5D-O5D
3	D	402[B]	NAP	C3D-C4D-C5D-O5D
3	D	402[A]	NAP	C4D-C5D-O5D-PN
2	A	401	FAD	C3B-C4B-C5B-O5B
2	D	401	FAD	O4B-C4B-C5B-O5B
3	D	402[A]	NAP	C1B-C2B-O2B-P2B
3	D	402[A]	NAP	C3D-C4D-C5D-O5D
2	G	401	FAD	O4B-C4B-C5B-O5B
2	A	401	FAD	PA-O3P-P-O5'
2	B	401	FAD	PA-O3P-P-O5'
2	D	401	FAD	P-O3P-PA-O5B
2	E	401	FAD	PA-O3P-P-O5'
2	F	401	FAD	PA-O3P-P-O5'
2	G	401	FAD	C2B-C1B-N9A-C8A
2	B	401	FAD	P-O3P-PA-O1A
3	C	402	NAP	PA-O3-PN-O2N
3	D	402[B]	NAP	PA-O3-PN-O2N
2	A	401	FAD	C5B-O5B-PA-O1A
2	A	401	FAD	C5B-O5B-PA-O3P
2	B	401	FAD	C5'-O5'-P-O1P
2	B	401	FAD	C5'-O5'-P-O3P
3	C	402	NAP	C5D-O5D-PN-O3
3	C	402	NAP	C5D-O5D-PN-O1N
3	C	402	NAP	C5D-O5D-PN-O2N
3	D	402[A]	NAP	C5B-O5B-PA-O1A
3	F	402	NAP	C5B-O5B-PA-O1A
3	F	402	NAP	C5B-O5B-PA-O2A
3	F	402	NAP	C5D-O5D-PN-O3
2	H	401	FAD	C4'-C5'-O5'-P
3	F	402	NAP	C4D-C5D-O5D-PN
3	C	402	NAP	C1B-C2B-O2B-P2B
3	C	402	NAP	O4B-C4B-C5B-O5B
2	G	401	FAD	C3B-C4B-C5B-O5B
3	C	402	NAP	C3B-C4B-C5B-O5B
3	D	402[A]	NAP	C2B-O2B-P2B-O1X
3	F	402	NAP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
2	E	401	FAD	P-O3P-PA-O1A
2	G	401	FAD	O4B-C1B-N9A-C8A
2	D	401	FAD	C4B-C5B-O5B-PA
2	D	401	FAD	PA-O3P-P-O1P
2	E	401	FAD	P-O3P-PA-O2A
2	F	401	FAD	P-O3P-PA-O1A
2	F	401	FAD	P-O3P-PA-O2A
2	G	401	FAD	P-O3P-PA-O2A
3	C	402	NAP	PA-O3-PN-O1N
3	F	402	NAP	PA-O3-PN-O2N
3	C	402	NAP	C2B-O2B-P2B-O3X
3	D	402[A]	NAP	C2B-O2B-P2B-O2X
3	D	402[A]	NAP	C2B-O2B-P2B-O3X
3	C	402	NAP	C2B-C1B-N9A-C8A
2	E	401	FAD	N10-C1'-C2'-O2'
3	D	402[B]	NAP	C2B-O2B-P2B-O1X
2	A	401	FAD	C2B-C1B-N9A-C8A
2	A	401	FAD	PA-O3P-P-O1P
2	H	401	FAD	P-O3P-PA-O2A
3	D	402[B]	NAP	PA-O3-PN-O1N
3	F	402	NAP	PA-O3-PN-O1N

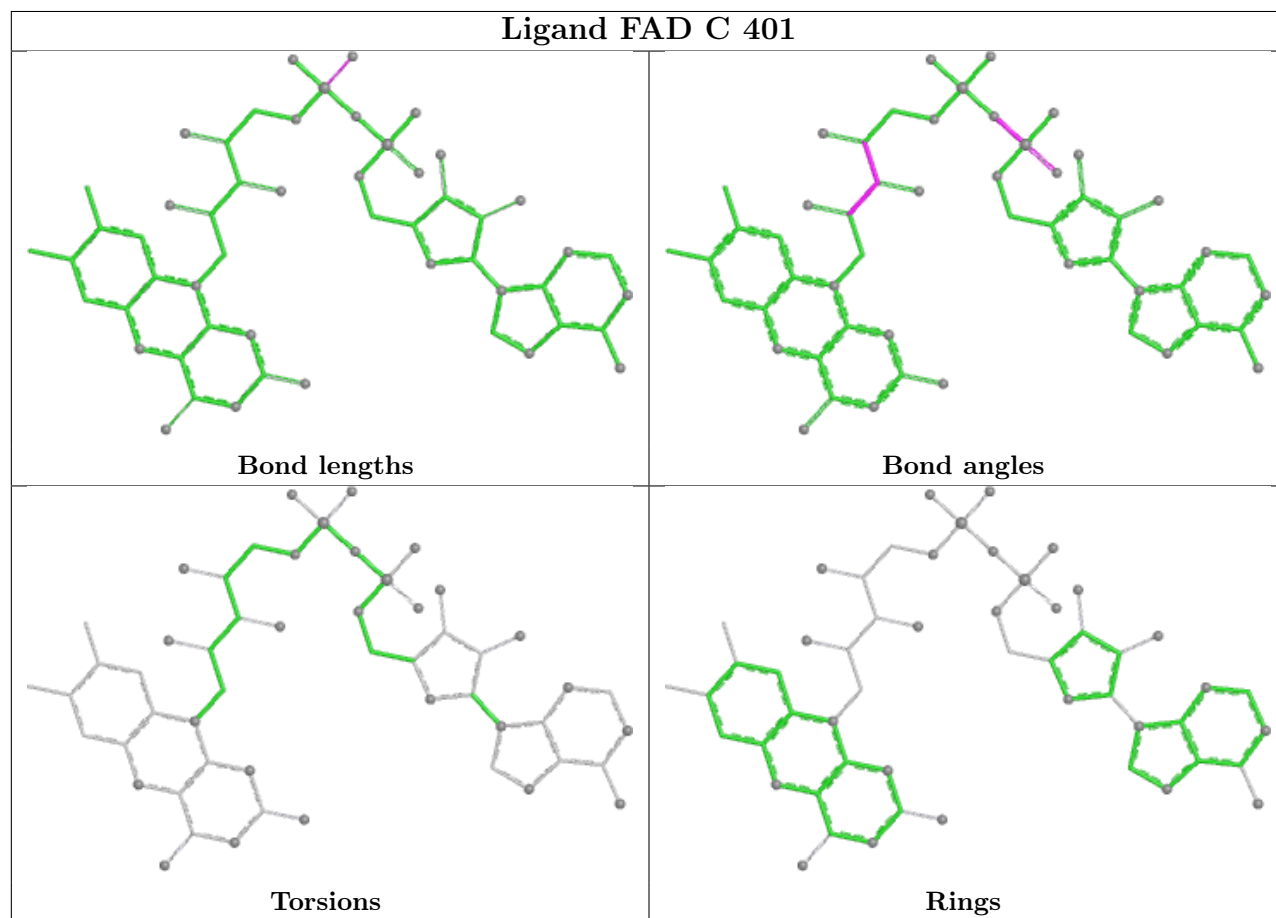
There are no ring outliers.

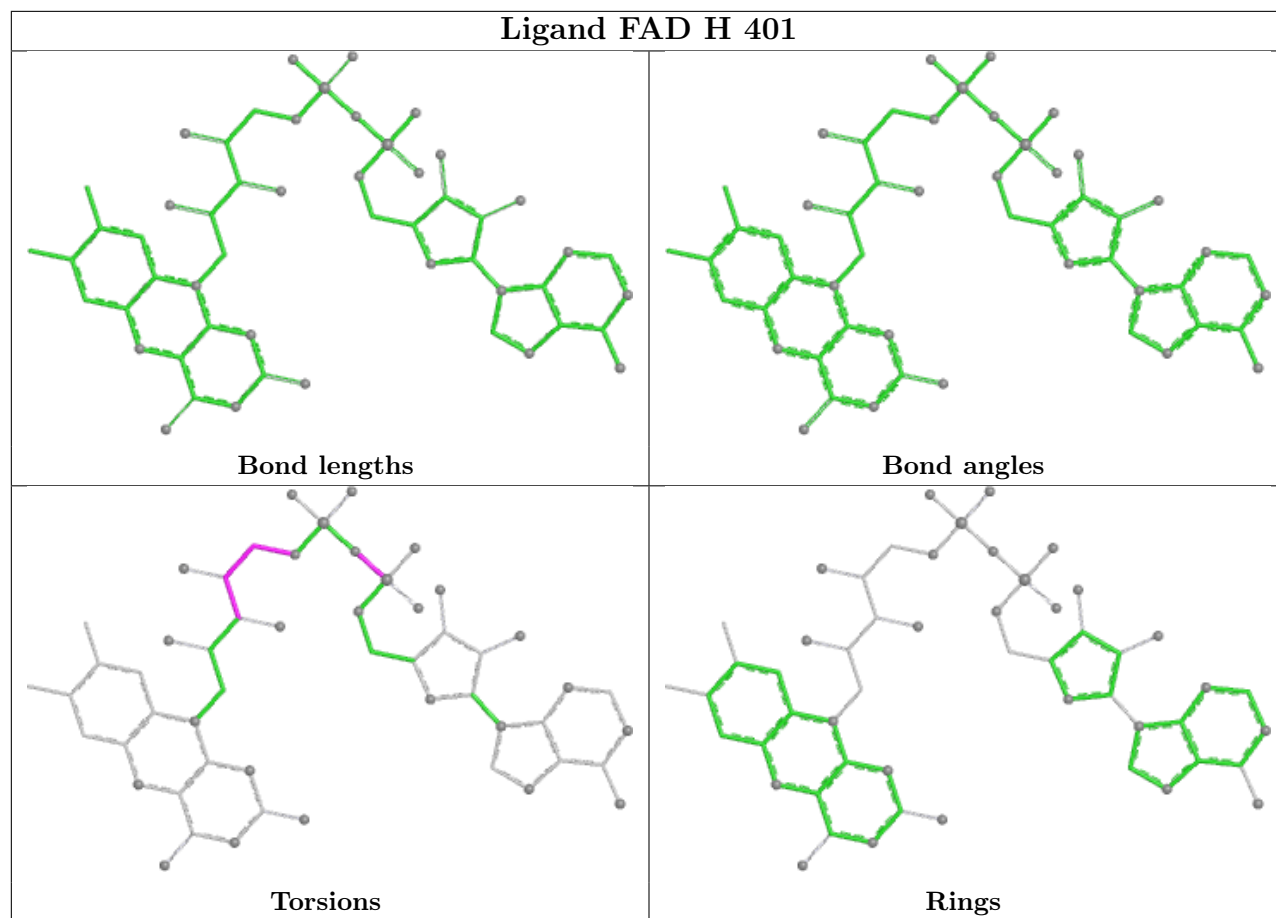
10 monomers are involved in 45 short contacts:

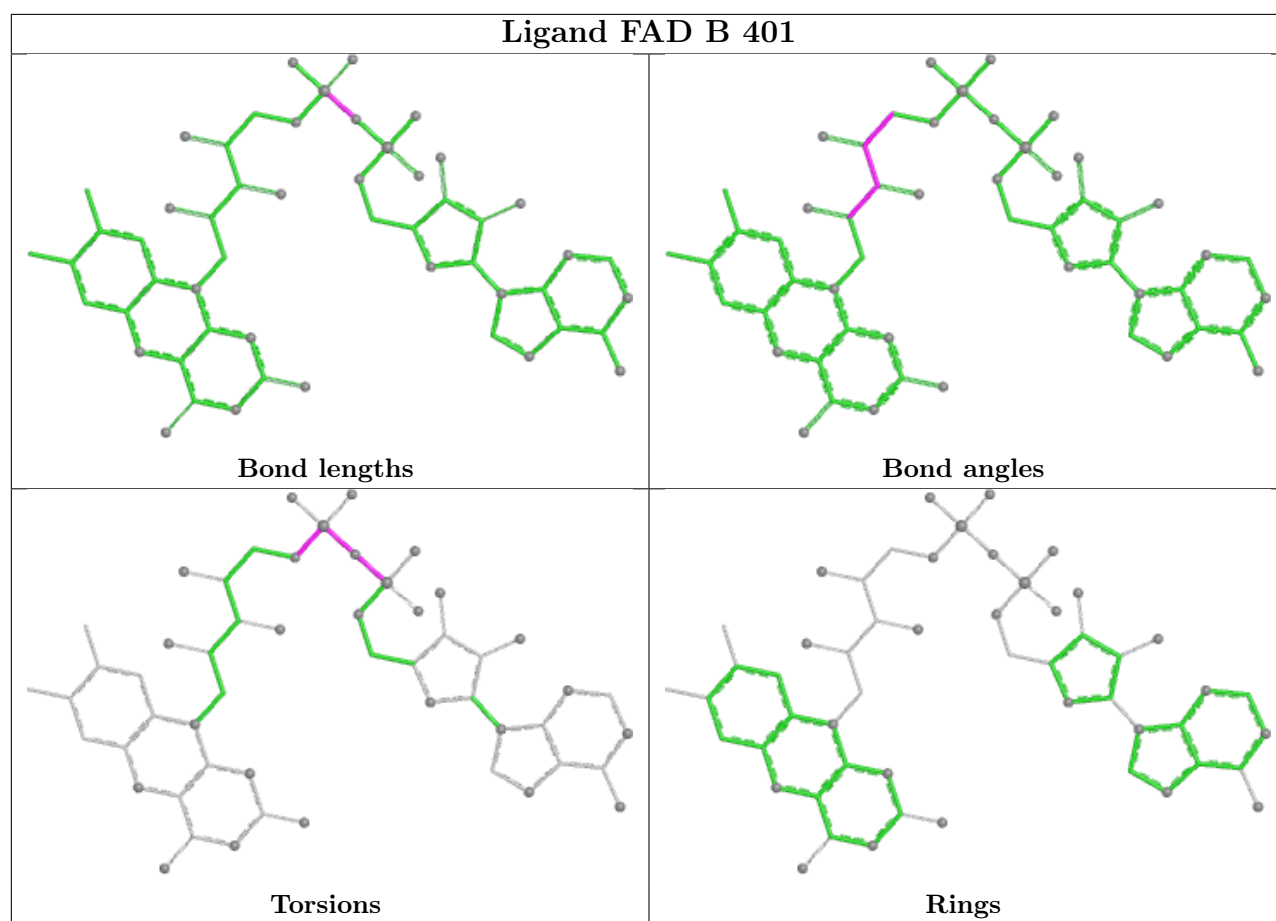
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	FAD	3	0
2	H	401	FAD	5	0
2	F	401	FAD	1	0
3	D	402[B]	NAP	7	0
3	F	402	NAP	6	0
2	D	401	FAD	2	0
2	G	401	FAD	4	0
3	C	402	NAP	4	0
2	A	401	FAD	3	0
3	D	402[A]	NAP	10	0

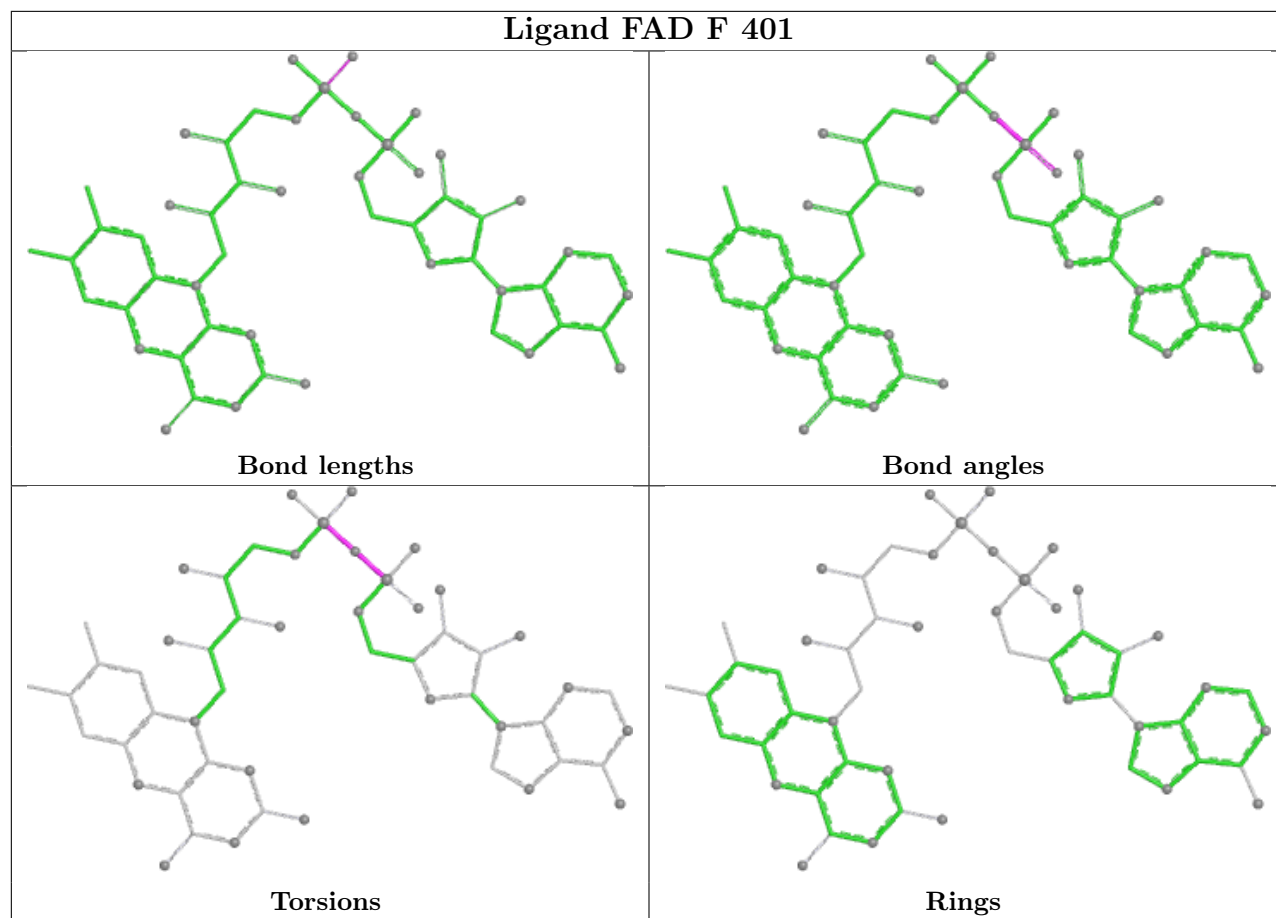
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

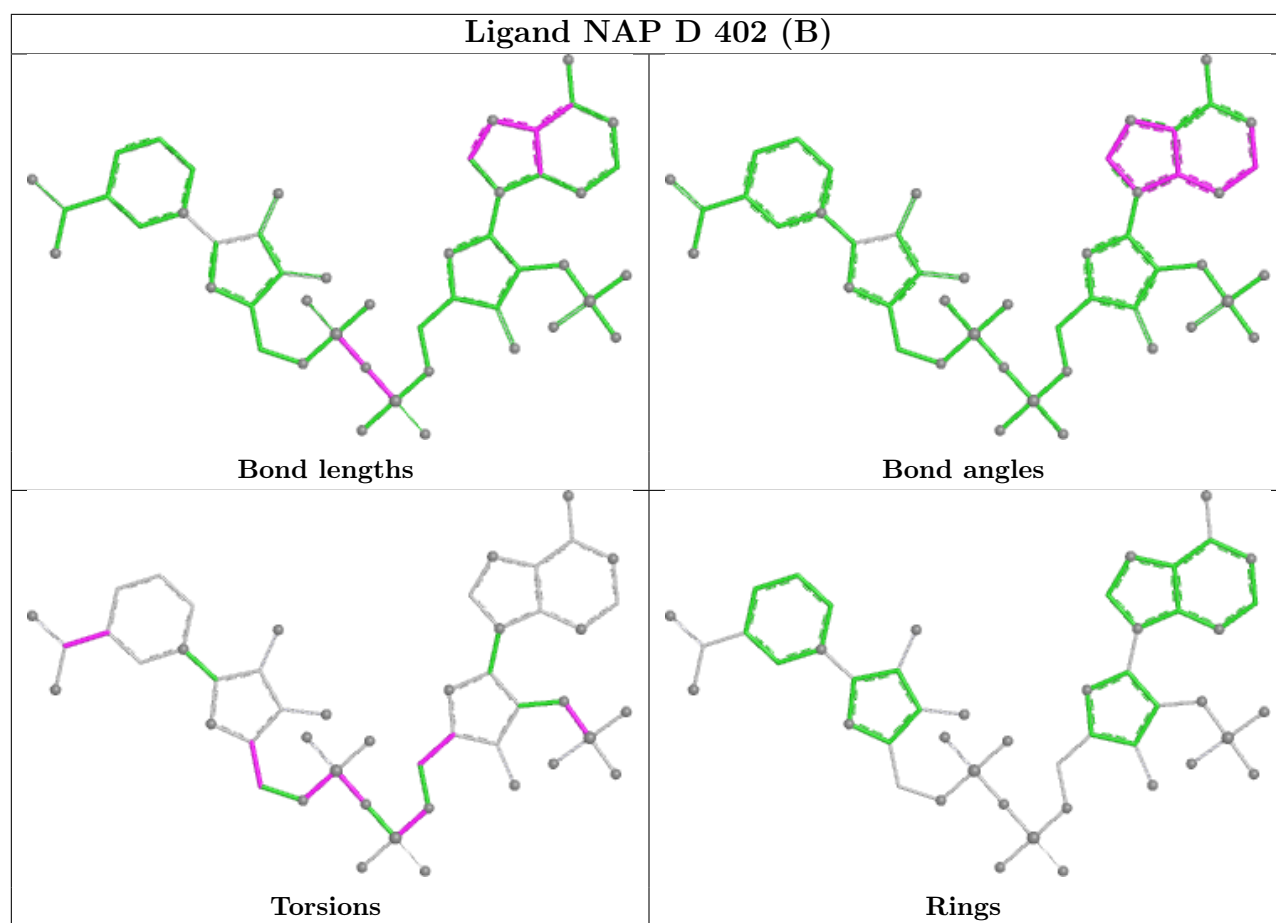
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

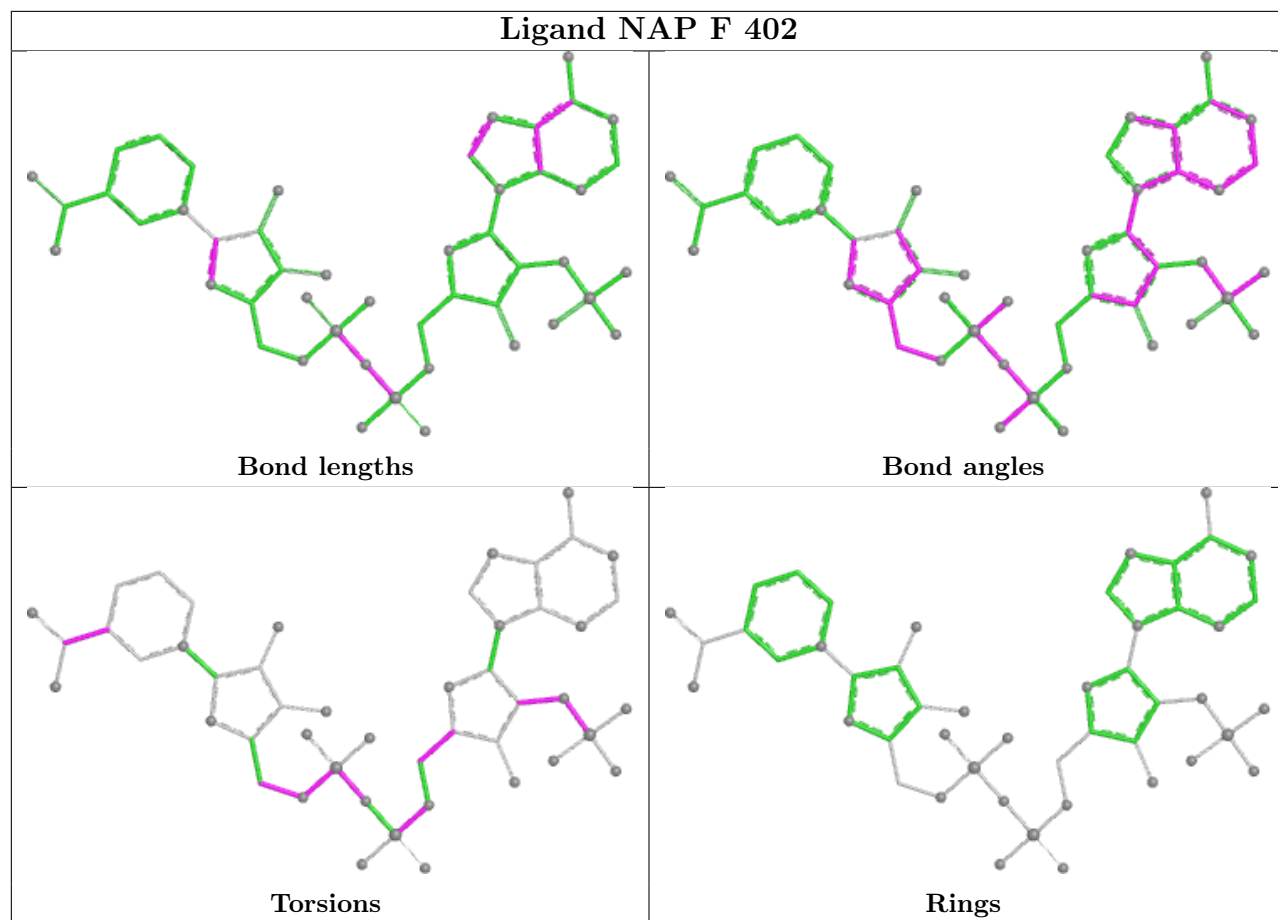


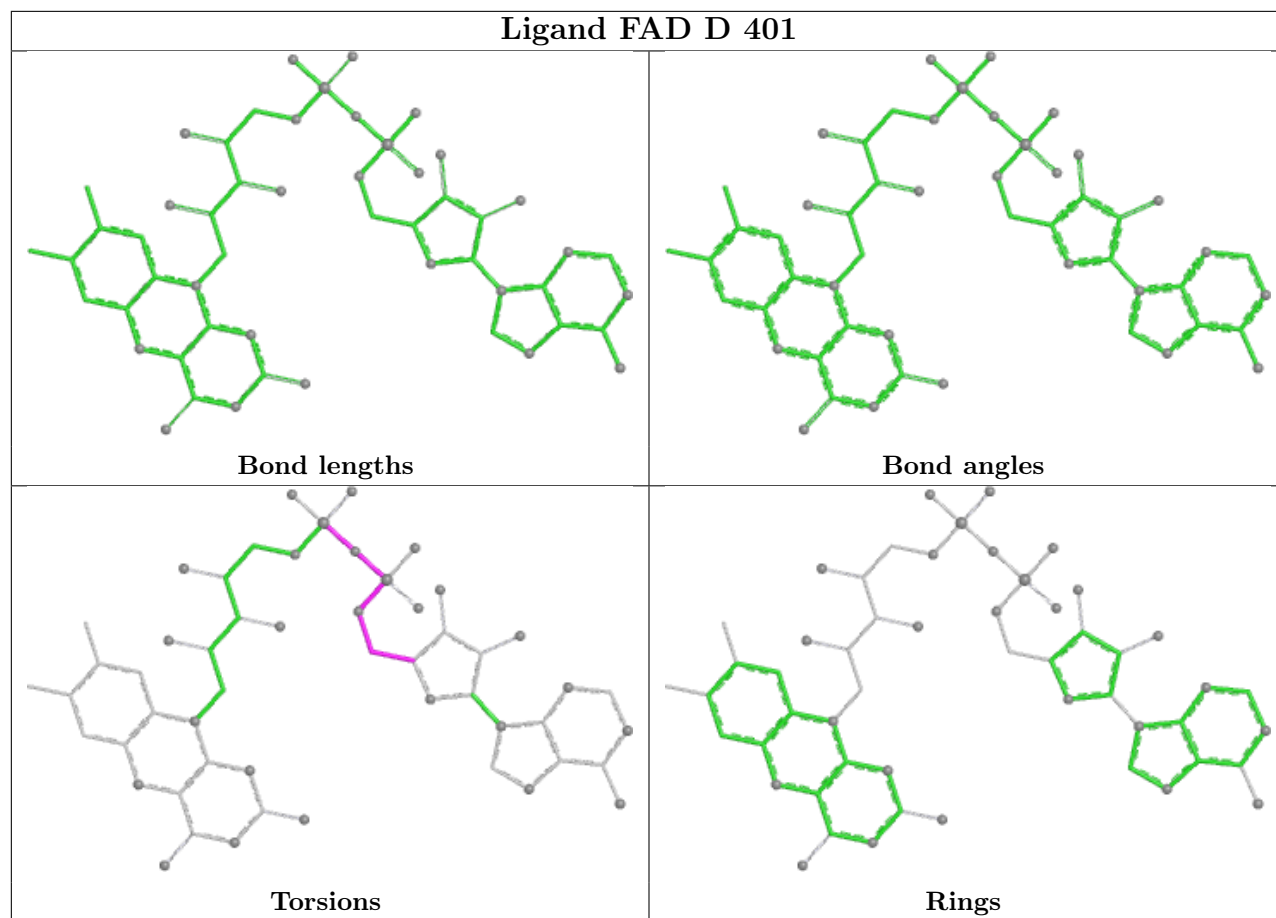


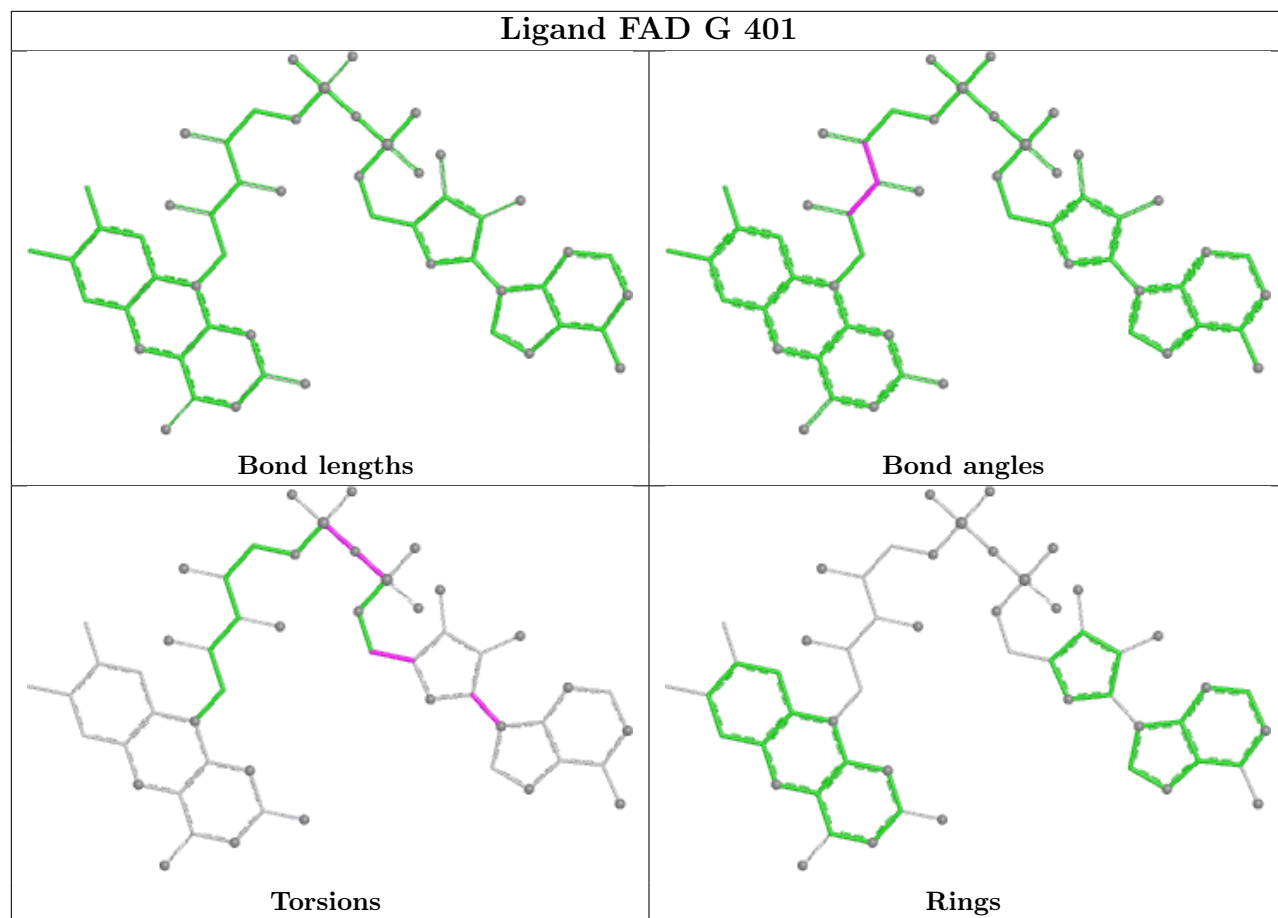


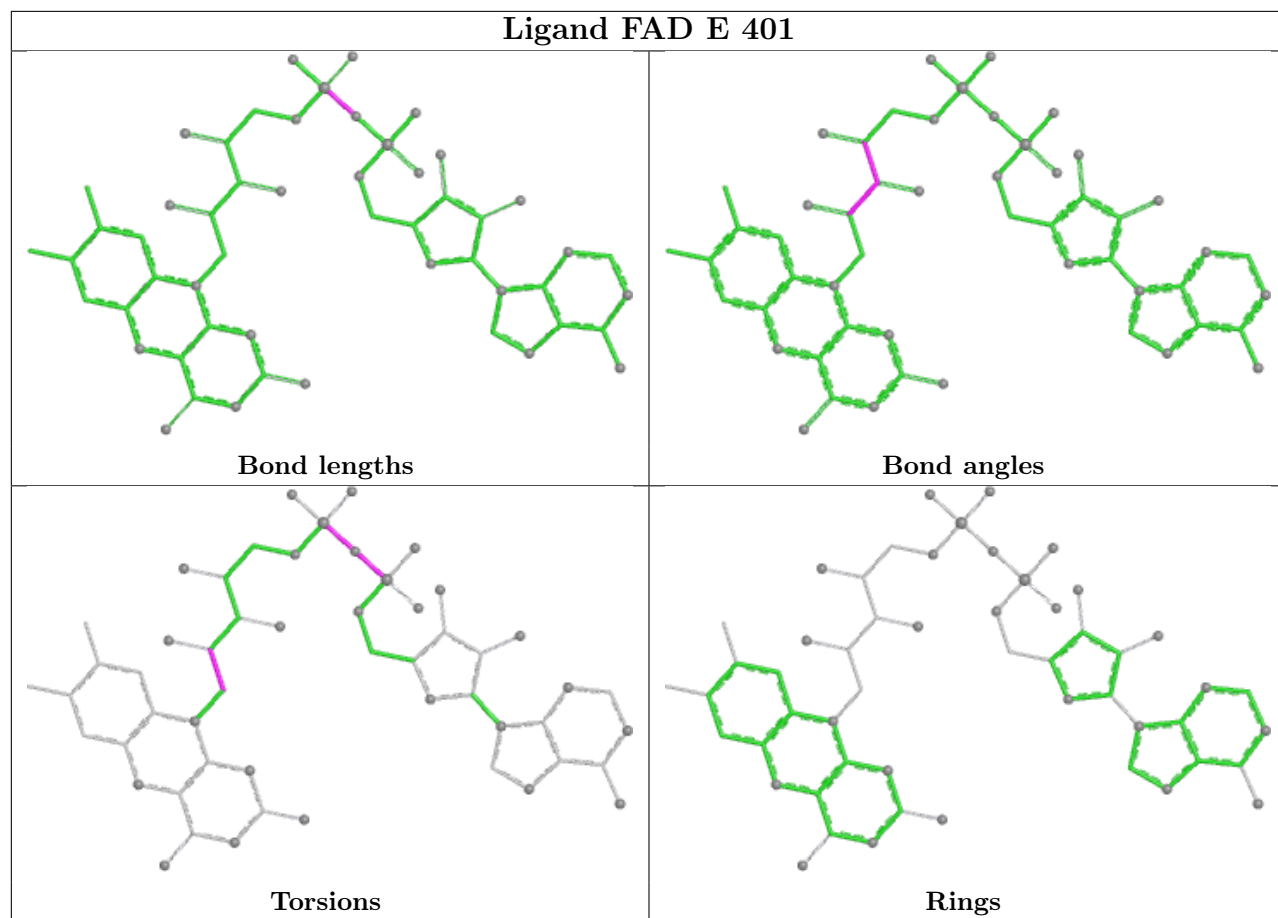


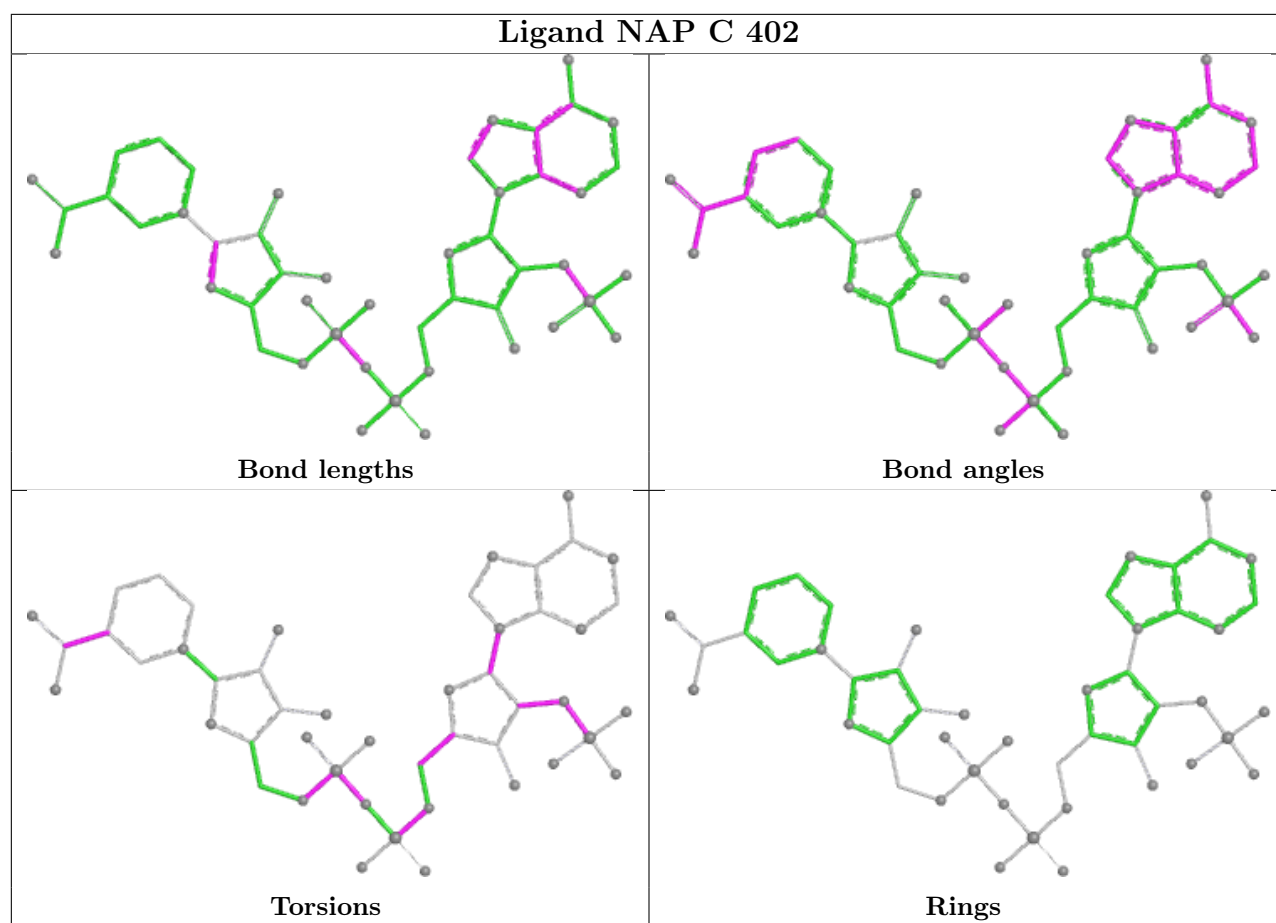


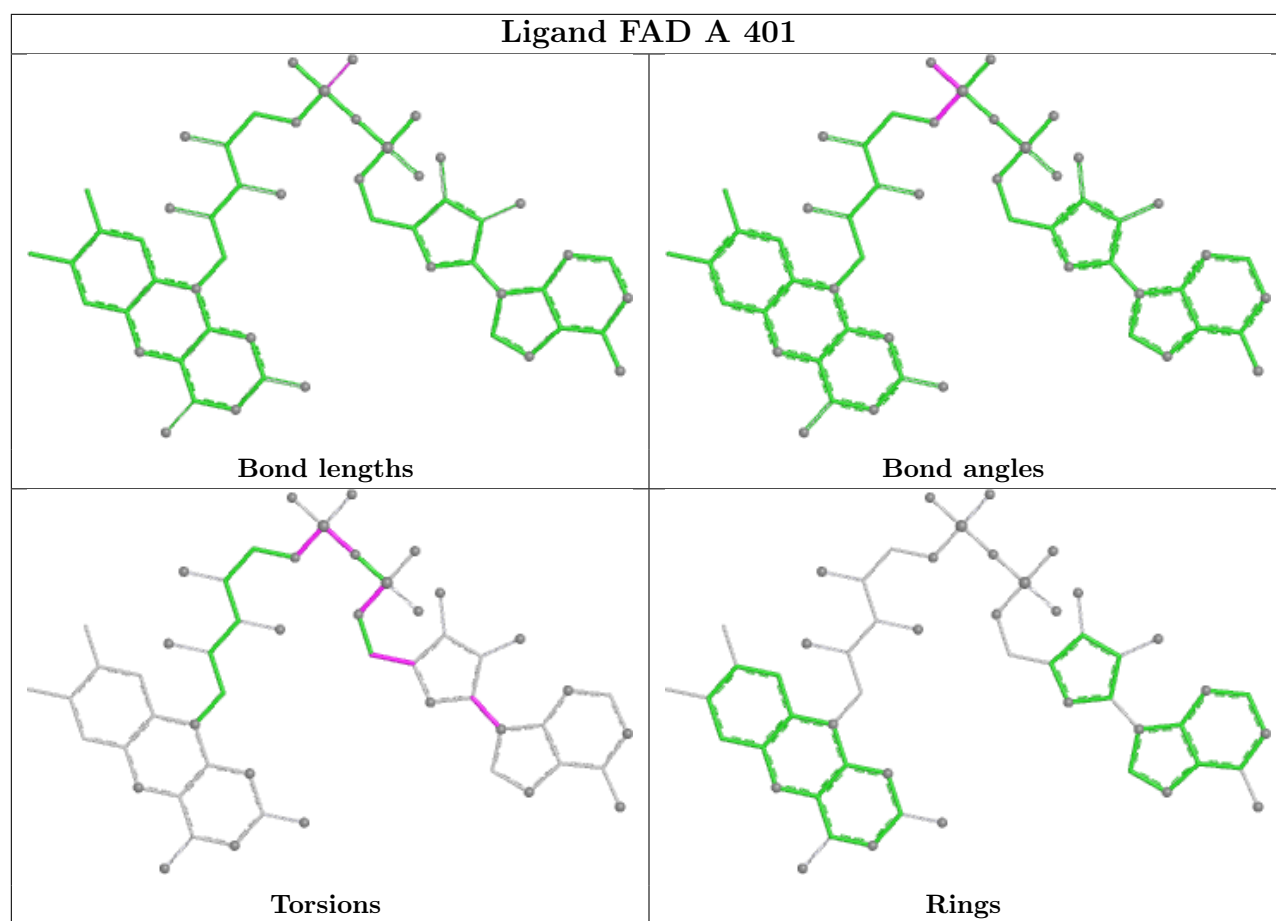


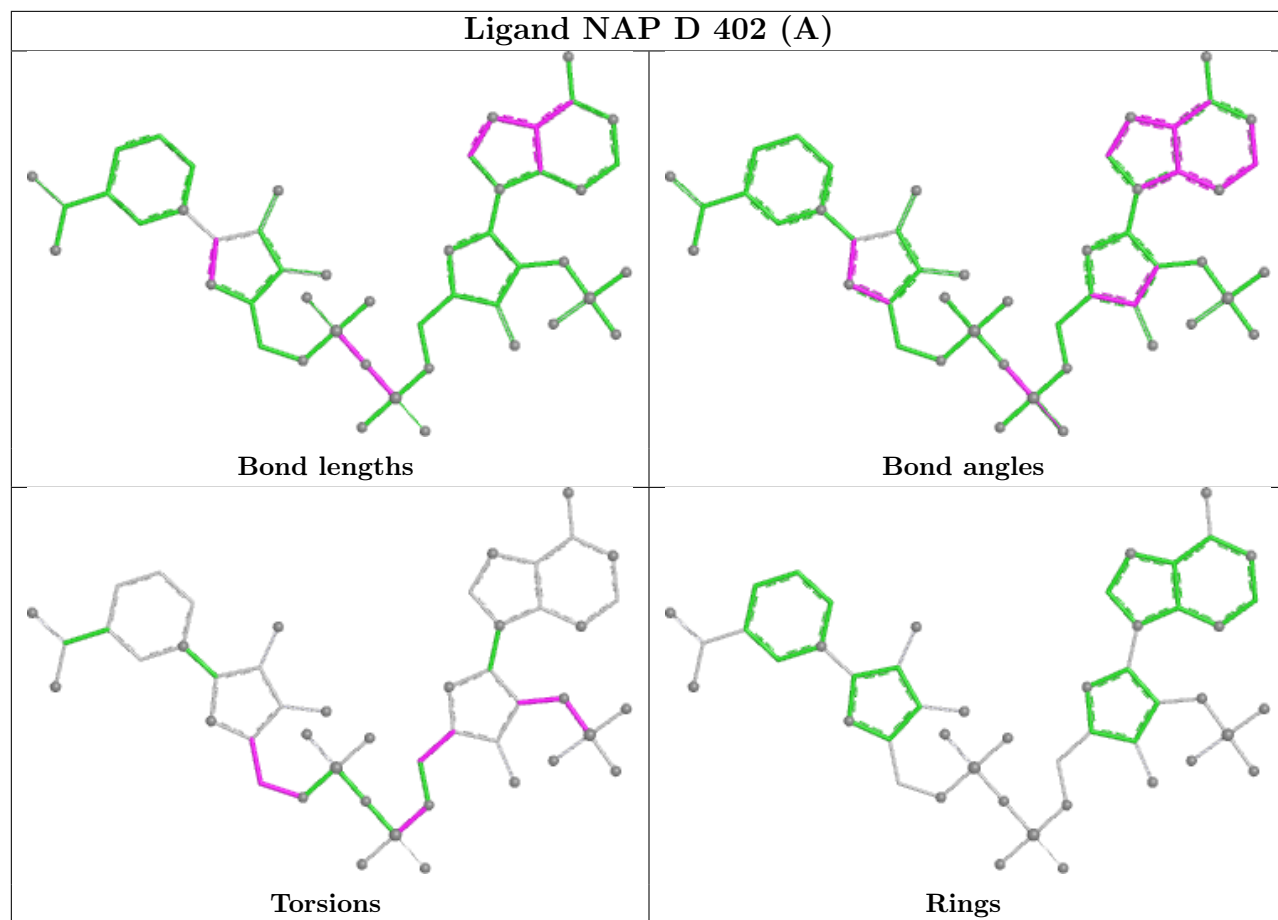












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/328 (98%)	-0.00	5 (1%) 72 64	28, 47, 71, 96	0
1	B	323/328 (98%)	0.16	6 (1%) 66 58	27, 50, 86, 104	0
1	C	323/328 (98%)	-0.14	2 (0%) 85 81	24, 39, 64, 100	1 (0%)
1	D	323/328 (98%)	-0.05	3 (0%) 81 75	18, 43, 74, 89	1 (0%)
1	E	323/328 (98%)	-0.11	4 (1%) 76 69	23, 40, 71, 112	1 (0%)
1	F	323/328 (98%)	0.04	3 (0%) 81 75	20, 45, 76, 93	2 (0%)
1	G	265/328 (80%)	2.14	121 (45%) 0 0	76, 113, 142, 171	0
1	H	323/328 (98%)	2.39	184 (56%) 0 0	71, 112, 154, 180	0
All	All	2526/2624 (96%)	0.52	328 (12%) 7 6	18, 50, 135, 180	5 (0%)

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	91	VAL	10.0
1	H	42	TYR	8.2
1	H	175	LEU	7.9
1	G	63	PRO	7.5
1	H	300	ASN	7.1
1	G	71	PRO	7.1
1	H	180	ALA	6.9
1	H	178	ALA	6.8
1	G	64	PHE	6.7
1	H	186	TYR	6.3
1	H	299	ALA	6.0
1	H	151	ALA	6.0
1	H	291	GLY	5.9
1	G	148	PHE	5.8
1	G	151	ALA	5.5
1	H	182	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	G	100	VAL	5.3
1	H	303	PHE	5.3
1	H	71	PRO	5.2
1	H	66	VAL	5.1
1	G	51	PHE	5.1
1	H	38	VAL	5.0
1	H	41	ILE	5.0
1	H	94	PHE	5.0
1	H	121	LEU	4.9
1	H	214	MET	4.8
1	H	189	GLY	4.8
1	G	289	ILE	4.6
1	H	269	PHE	4.6
1	H	311	GLY	4.6
1	D	296	GLY	4.5
1	G	115	VAL	4.5
1	B	299	ALA	4.5
1	H	218	ALA	4.5
1	G	216	PHE	4.4
1	G	92	ASN	4.4
1	H	68	GLU	4.4
1	H	264	ILE	4.4
1	H	203	PHE	4.3
1	G	62	VAL	4.3
1	H	257	LEU	4.3
1	H	127	TYR	4.3
1	G	302	ILE	4.2
1	G	13	PRO	4.2
1	H	172	ALA	4.2
1	A	298	ASP	4.2
1	H	304	ILE	4.2
1	H	282	THR	4.1
1	H	274	MET	4.1
1	G	269	PHE	4.1
1	H	64	PHE	4.1
1	E	300	ASN	4.1
1	H	126	GLY	4.1
1	G	95	GLU	4.1
1	G	152	HIS	4.1
1	H	170	ASP	4.0
1	G	147	TYR	4.0
1	G	154	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	239	ILE	4.0
1	H	289	ILE	4.0
1	H	160	VAL	4.0
1	H	16	LEU	3.9
1	G	303	PHE	3.9
1	G	66	VAL	3.9
1	G	109	ILE	3.9
1	H	185	LEU	3.8
1	G	309	PHE	3.8
1	H	174	GLU	3.8
1	G	84	VAL	3.8
1	G	32	ILE	3.8
1	H	309	PHE	3.8
1	H	123	ILE	3.8
1	H	70	LYS	3.8
1	G	19	ALA	3.8
1	G	16	LEU	3.8
1	G	34	LYS	3.7
1	G	29	THR	3.7
1	H	67	GLU	3.7
1	G	290	ALA	3.7
1	H	234	GLY	3.7
1	H	39	GLU	3.7
1	H	53	SER	3.6
1	G	301	THR	3.6
1	H	46	THR	3.6
1	G	8	ILE	3.6
1	G	37	VAL	3.6
1	H	296	GLY	3.6
1	G	112	THR	3.6
1	G	294	ALA	3.5
1	H	295	ALA	3.5
1	H	260	VAL	3.5
1	H	179	GLY	3.5
1	H	37	VAL	3.5
1	H	262	ILE	3.5
1	H	163	GLY	3.4
1	G	9	ILE	3.4
1	H	199	ILE	3.4
1	G	97	VAL	3.4
1	G	134	LEU	3.4
1	G	27	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	115	VAL	3.4
1	G	273	PRO	3.4
1	H	63	PRO	3.3
1	G	47	HIS	3.3
1	H	65	ILE	3.3
1	H	69	SER	3.3
1	H	159	VAL	3.3
1	H	184	VAL	3.3
1	H	173	LEU	3.3
1	H	216	PHE	3.3
1	H	49	THR	3.3
1	H	128	TYR	3.3
1	H	52	SER	3.3
1	H	273	PRO	3.3
1	G	57	LEU	3.3
1	H	275	TYR	3.2
1	G	65	ILE	3.2
1	H	290	ALA	3.2
1	G	266	THR	3.2
1	G	243	TYR	3.2
1	H	77	LEU	3.2
1	H	51	PHE	3.2
1	H	319	LEU	3.2
1	H	270	GLY	3.2
1	G	94	PHE	3.2
1	G	271	THR	3.2
1	H	301	THR	3.2
1	H	155	PHE	3.1
1	G	11	GLY	3.1
1	G	82	GLU	3.1
1	H	305	GLU	3.1
1	H	187	ARG	3.1
1	G	220	VAL	3.1
1	H	233	ASN	3.1
1	H	302	ILE	3.1
1	H	183	THR	3.1
1	H	266	THR	3.1
1	H	125	THR	3.1
1	B	294	ALA	3.0
1	H	98	LEU	3.0
1	G	7	ILE	3.0
1	C	268	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	76	ALA	3.0
1	G	50	PHE	3.0
1	G	123	ILE	3.0
1	H	161	ILE	3.0
1	G	267	ASN	3.0
1	H	217	ASN	3.0
1	H	297	ASN	3.0
1	G	68	GLU	3.0
1	H	292	VAL	3.0
1	A	300	ASN	3.0
1	G	313	ILE	2.9
1	H	293	ILE	2.9
1	H	44	TYR	2.9
1	G	2	GLN	2.9
1	H	245	PHE	2.9
1	G	90	LYS	2.9
1	G	10	GLY	2.9
1	G	217	ASN	2.9
1	G	101	LYS	2.9
1	H	279	THR	2.9
1	H	294	ALA	2.9
1	H	110	THR	2.9
1	H	162	ILE	2.9
1	G	96	GLU	2.9
1	H	101	LYS	2.9
1	H	78	VAL	2.9
1	H	133	THR	2.9
1	H	204	THR	2.9
1	G	70	LYS	2.8
1	G	254	TYR	2.8
1	G	99	THR	2.8
1	G	257	LEU	2.8
1	B	293	ILE	2.8
1	G	261	GLY	2.8
1	G	1	MET	2.8
1	H	60	GLY	2.8
1	H	45	PRO	2.8
1	H	313	ILE	2.8
1	H	131	HIS	2.8
1	H	152	HIS	2.8
1	H	34	LYS	2.8
1	H	122	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	153	PRO	2.8
1	G	157	GLN	2.7
1	G	139	ALA	2.7
1	H	191	TYR	2.7
1	G	142	PRO	2.7
1	H	207	VAL	2.7
1	G	89	LEU	2.7
1	H	50	PHE	2.7
1	H	272	ALA	2.7
1	G	128	TYR	2.7
1	H	288	TYR	2.7
1	H	97	VAL	2.7
1	H	30	LEU	2.7
1	H	254	TYR	2.7
1	G	133	THR	2.7
1	H	181	ASN	2.7
1	G	78	VAL	2.6
1	G	277	LYS	2.6
1	H	206	LEU	2.6
1	H	120	PHE	2.6
1	H	280	TYR	2.6
1	H	57	LEU	2.6
1	H	62	VAL	2.6
1	H	212	ILE	2.6
1	G	114	ASP	2.6
1	H	156	ASP	2.6
1	G	116	TYR	2.6
1	G	155	PHE	2.6
1	H	80	TYR	2.6
1	H	100	VAL	2.6
1	H	40	SER	2.5
1	H	259	SER	2.5
1	G	98	LEU	2.5
1	H	164	GLY	2.5
1	H	252	PRO	2.5
1	G	239	ILE	2.5
1	G	260	VAL	2.5
1	H	31	ILE	2.5
1	E	299	ALA	2.5
1	H	61	ASP	2.5
1	H	4	VAL	2.5
1	H	284	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	116	TYR	2.5
1	E	269	PHE	2.5
1	G	38	VAL	2.5
1	H	48	GLN	2.5
1	G	292	VAL	2.5
1	G	76	ALA	2.5
1	H	165	LYS	2.4
1	H	177	LYS	2.4
1	H	205	ALA	2.4
1	G	46	THR	2.4
1	H	306	ASN	2.4
1	H	314	ILE	2.4
1	H	91	VAL	2.4
1	H	3	LYS	2.4
1	G	18	ALA	2.4
1	H	130	GLN	2.4
1	H	224	THR	2.4
1	G	30	LEU	2.4
1	H	142	PRO	2.4
1	H	153	PRO	2.4
1	G	270	GLY	2.4
1	H	188	GLY	2.4
1	G	113	LYS	2.4
1	G	322	LYS	2.4
1	G	69	SER	2.4
1	H	171	ALA	2.4
1	G	80	TYR	2.4
1	H	230	TYR	2.4
1	H	47	HIS	2.4
1	H	240	HIS	2.4
1	H	318	MET	2.4
1	G	121	LEU	2.4
1	G	36	ASN	2.4
1	H	223	ILE	2.4
1	G	264	ILE	2.3
1	H	109	ILE	2.3
1	H	148	PHE	2.3
1	F	298	ASP	2.3
1	H	124	ALA	2.3
1	A	264	ILE	2.3
1	H	29	THR	2.3
1	H	277	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	252	PRO	2.3
1	H	220	VAL	2.3
1	G	245	PHE	2.3
1	G	22	GLN	2.3
1	G	56	LYS	2.3
1	G	280	TYR	2.3
1	G	150	GLU	2.3
1	H	112	THR	2.3
1	H	211	LYS	2.2
1	B	267	ASN	2.2
1	F	267	ASN	2.2
1	H	149	LYS	2.2
1	H	283	ASN	2.2
1	D	264	ILE	2.2
1	G	244	VAL	2.2
1	G	12	GLY	2.2
1	G	145	PHE	2.2
1	H	322	LYS	2.2
1	H	36	ASN	2.2
1	H	213	ASP	2.2
1	H	228	VAL	2.2
1	H	232	VAL	2.2
1	F	60	GLY	2.2
1	G	42	TYR	2.2
1	G	221	THR	2.2
1	H	281	GLU	2.2
1	H	195	ILE	2.1
1	B	300	ASN	2.1
1	G	6	SER	2.1
1	H	176	GLU	2.1
1	H	7	ILE	2.1
1	H	298	ASP	2.1
1	E	51	PHE	2.1
1	H	154	TYR	2.1
1	H	287	CYS	2.1
1	G	87	HIS	2.1
1	G	4	VAL	2.1
1	H	13	PRO	2.1
1	A	296	GLY	2.1
1	G	107	PHE	2.1
1	G	110	THR	2.1
1	G	272	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	32	ILE	2.1
1	H	95	GLU	2.1
1	B	323	GLN	2.1
1	G	77	LEU	2.1
1	C	266	THR	2.1
1	G	67	GLU	2.1
1	H	215	GLU	2.1
1	H	6	SER	2.0
1	G	75	GLN	2.0
1	H	84	VAL	2.0
1	H	285	GLU	2.0
1	H	316	GLN	2.0
1	A	105	ASN	2.0
1	D	187	ARG	2.0
1	G	129	GLY	2.0
1	G	3	LYS	2.0
1	G	305	GLU	2.0
1	H	56	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

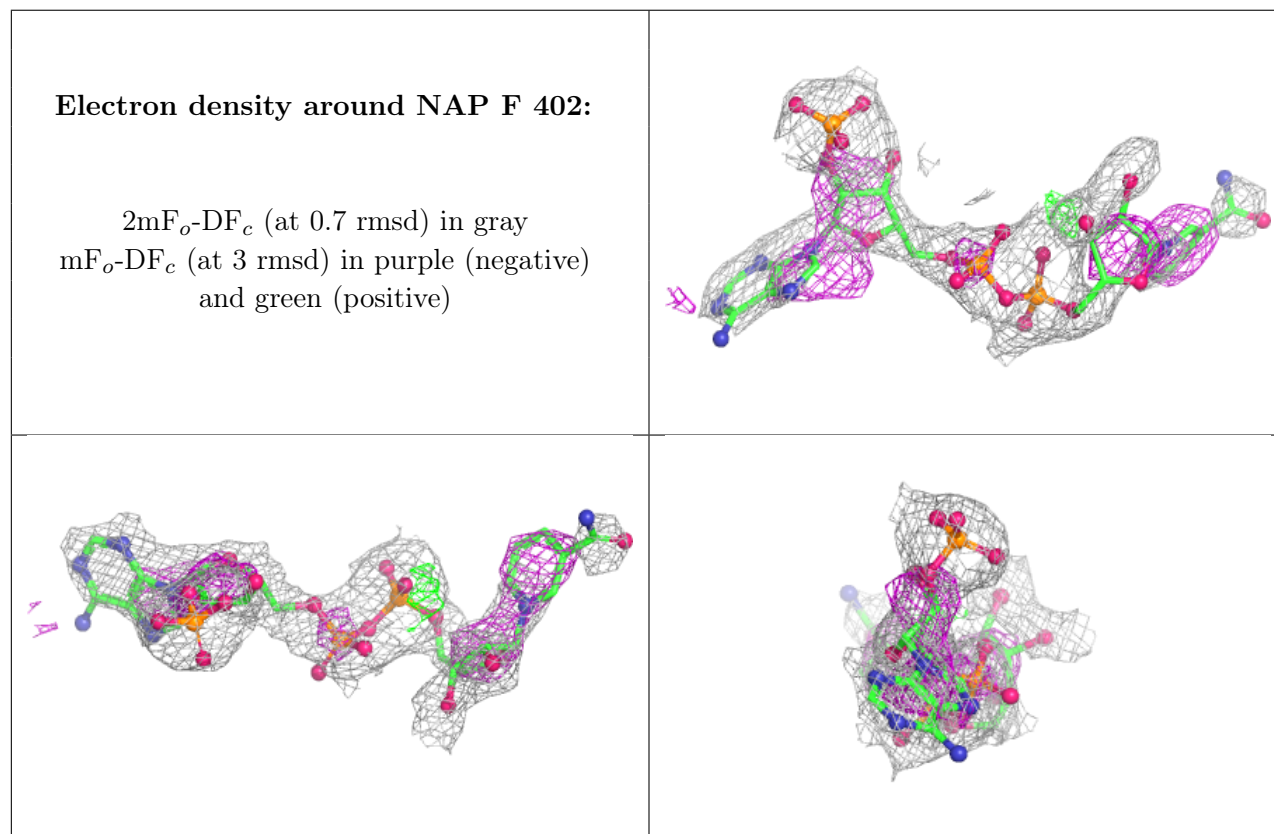
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAP	F	402	48/48	0.61	0.17	53,68,85,96	0
2	FAD	H	401	53/53	0.62	0.20	92,114,133,136	0
3	NAP	D	402[B]	48/48	0.64	0.21	40,55,65,67	48
3	NAP	D	402[A]	48/48	0.64	0.21	38,56,64,68	48
2	FAD	G	401	53/53	0.77	0.17	73,94,100,103	0

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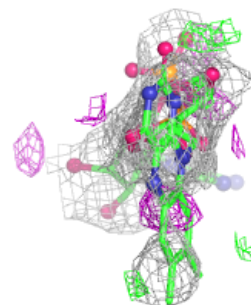
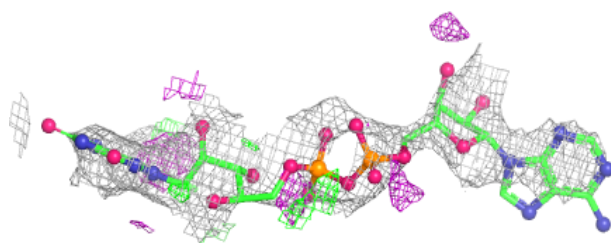
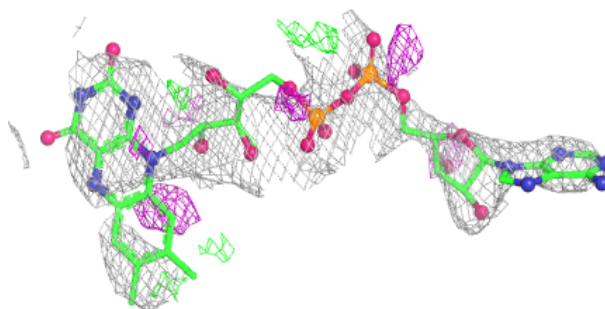
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	C	402	48/48	0.81	0.13	41,53,62,70	0
2	FAD	A	401	53/53	0.95	0.07	29,39,45,47	0
2	FAD	B	401	53/53	0.95	0.09	37,44,54,64	0
2	FAD	D	401	53/53	0.96	0.08	28,35,41,46	0
2	FAD	F	401	53/53	0.96	0.08	32,39,44,49	0
2	FAD	E	401	53/53	0.97	0.06	24,33,39,42	0
2	FAD	C	401	53/53	0.97	0.07	24,35,40,43	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.

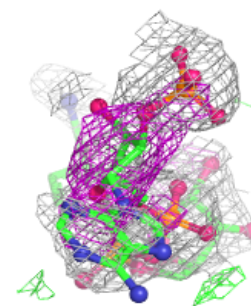
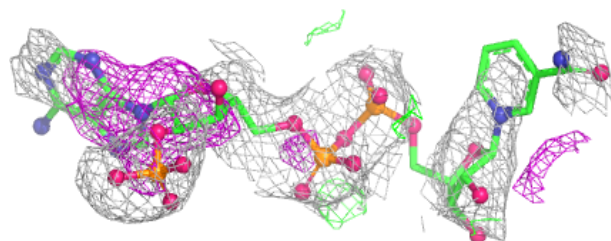
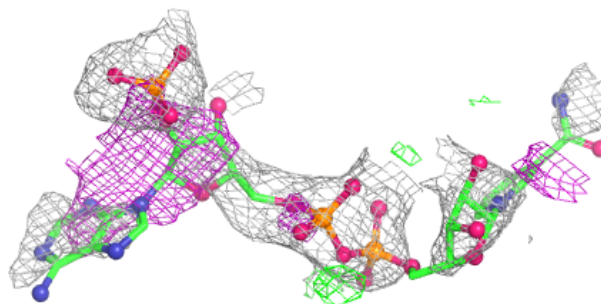


Electron density around FAD H 401:

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

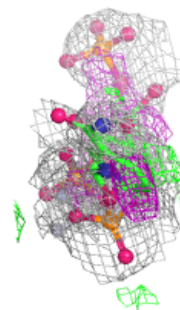
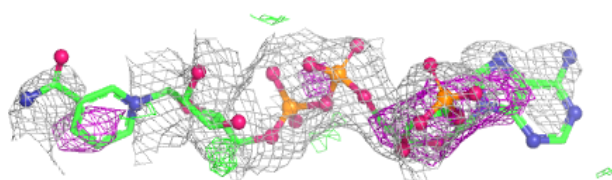
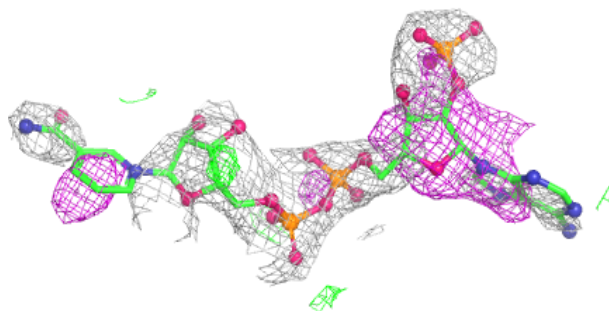
**Electron density around NAP D 402 (B):**

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

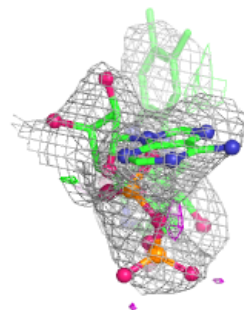
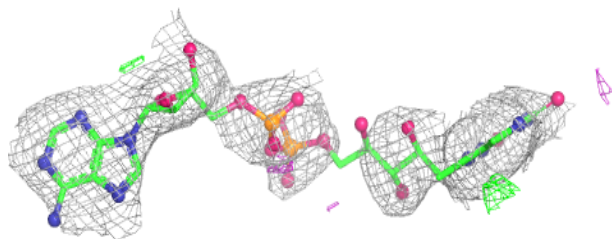
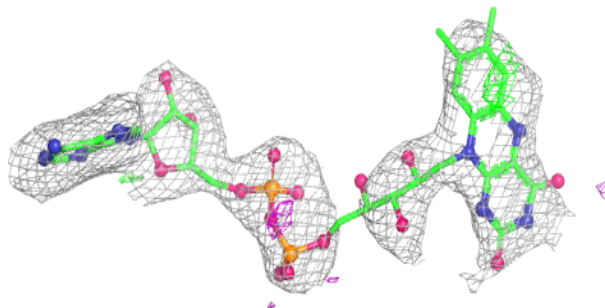


Electron density around NAP D 402 (A):

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

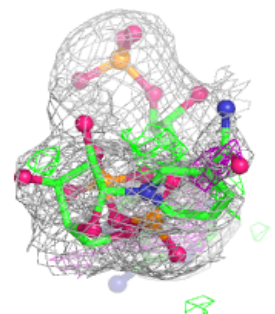
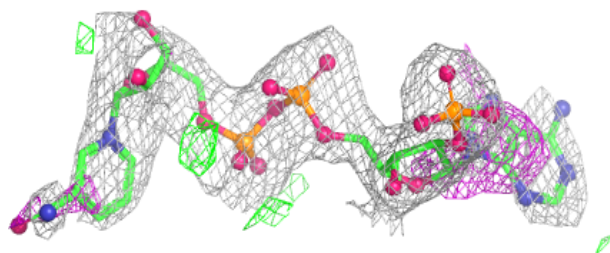
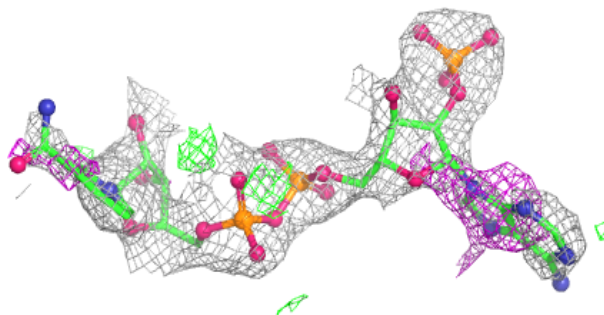
**Electron density around FAD G 401:**

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

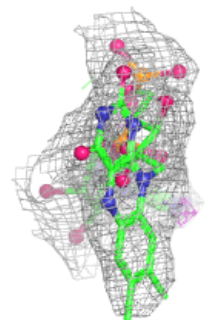
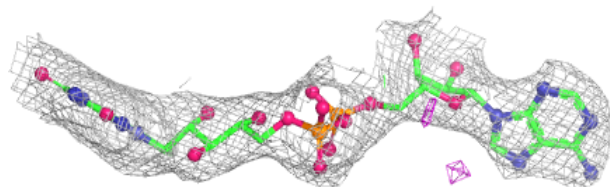
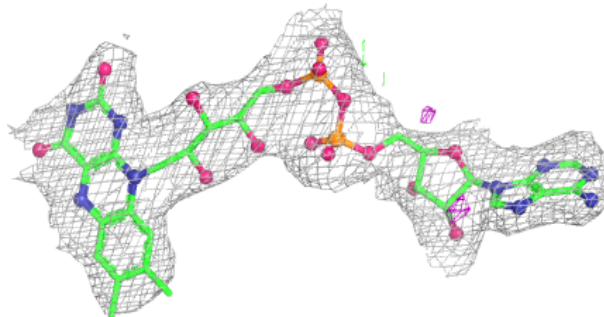


Electron density around NAP C 402:

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

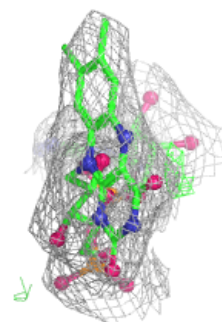
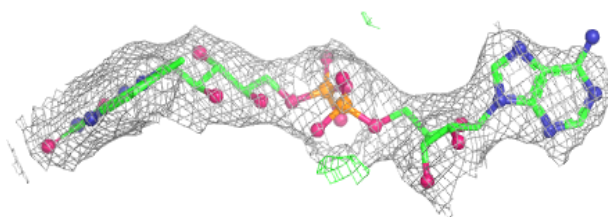
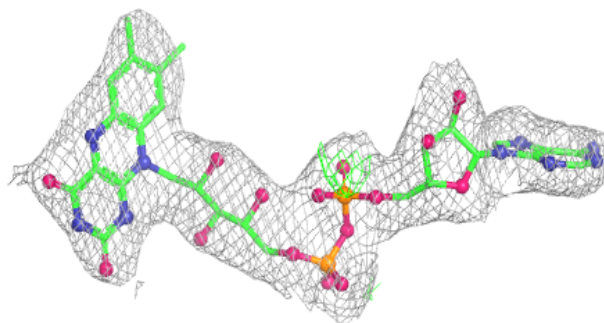
**Electron density around FAD A 401:**

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

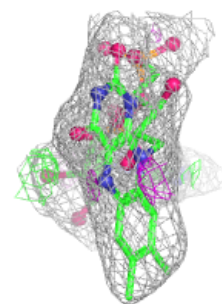
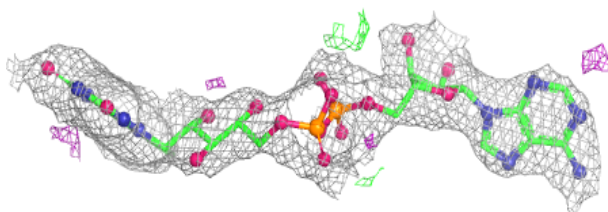
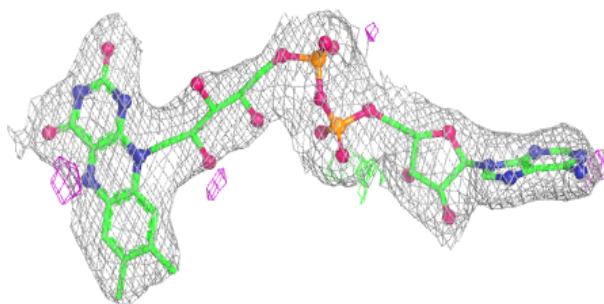


Electron density around FAD B 401:

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

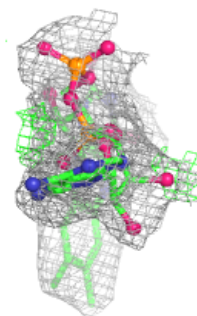
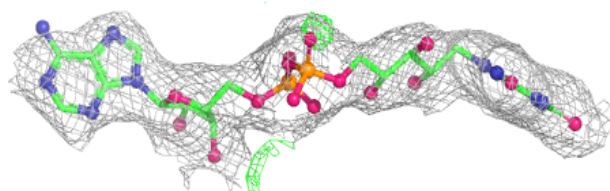
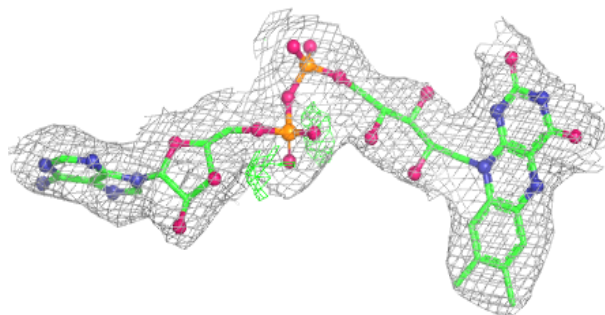
**Electron density around FAD D 401:**

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

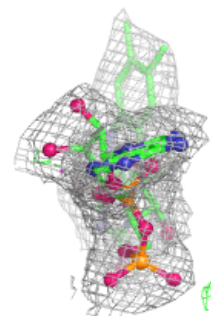
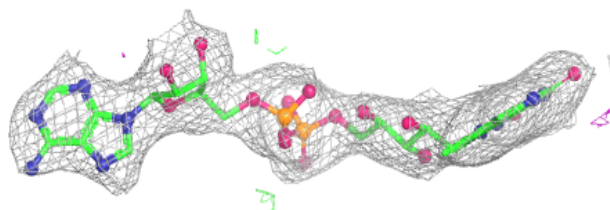
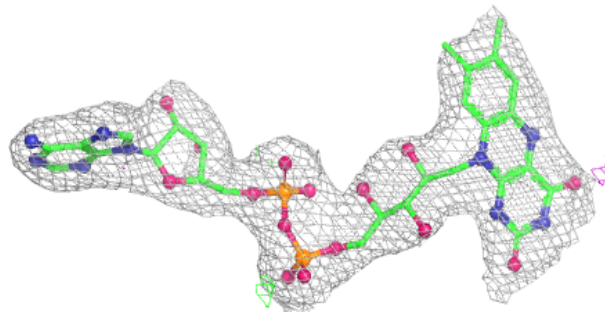


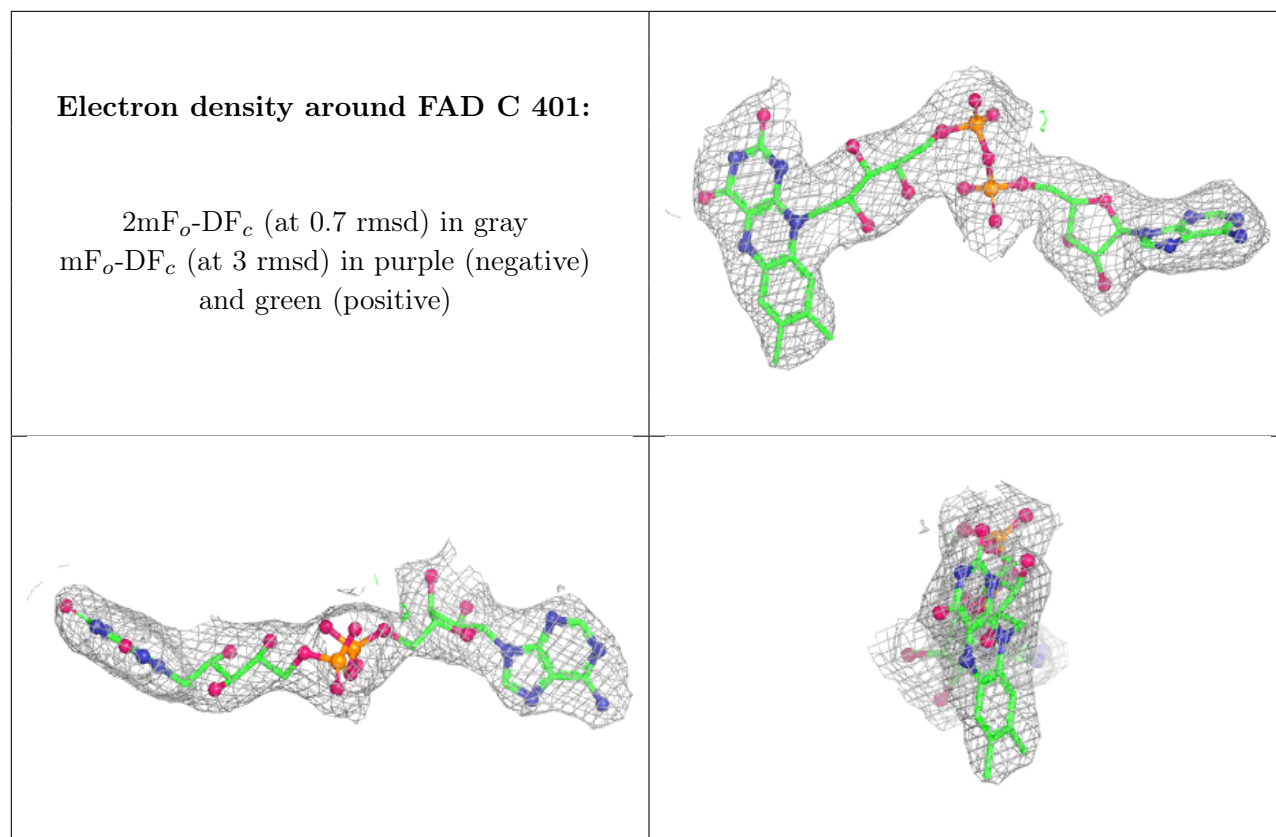
Electron density around FAD F 401:

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

**Electron density around FAD 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 [i](#)

There are no such residues in this entry.