



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:52 AM UTC

PDB ID : 1KBQ / pdb_00001kbq
Title : Complex of Human NAD(P)H quinone Oxidoreductase with 5-methoxy-1,2-dimethyl-3-(4-nitrophenoxyethyl)indole-4,7-dione (ES936)
Authors : Faig, M.; Bianchet, M.A.; Amzel, L.M.
Deposited on : 2001-11-06
Resolution : 1.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

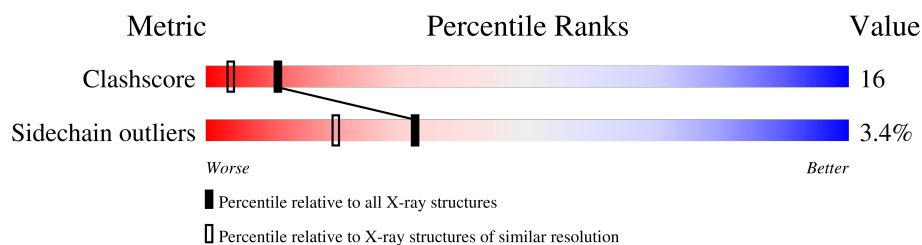
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8479 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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 $\leq 5\%$.

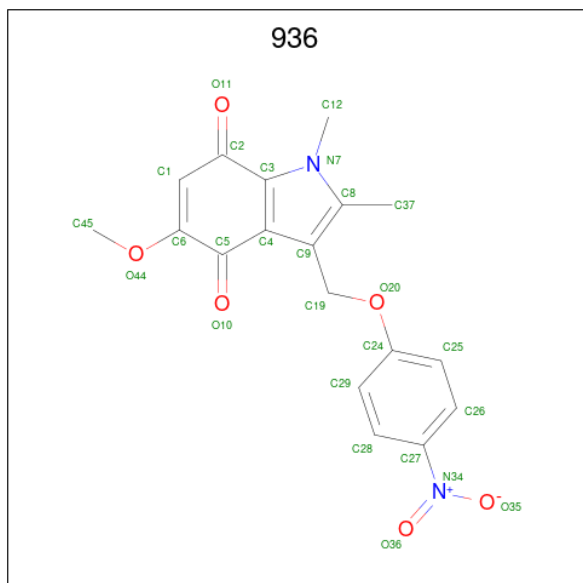
Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	273	
1	B	273	
1	C	273	
1	D	273	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is 5-METHOXY-1,2-DIMETHYL-3-(4-NITROPHENOXYMETHYL)INDOLE-4,7-DIONE (CCD ID: 936) (formula: $C_{18}H_{16}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	18	2	6		
3	B	1	Total	C	N	O	0	0
			26	18	2	6		
3	C	1	Total	C	N	O	0	0
			26	18	2	6		
3	D	1	Total	C	N	O	0	0
			26	18	2	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total	O	0	0
			129	129		
4	B	144	Total	O	0	0
			144	144		
4	C	114	Total	O	0	0
			114	114		

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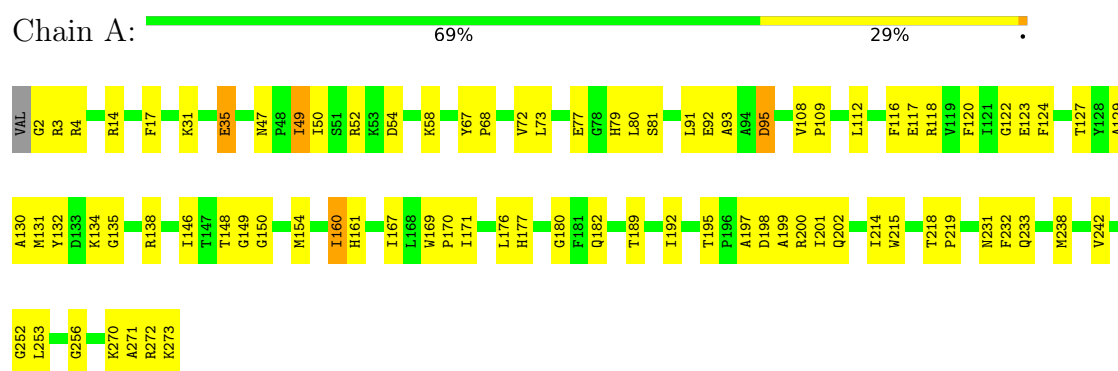
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	127	Total 127	O 127	0	0

3 Residue-property plots

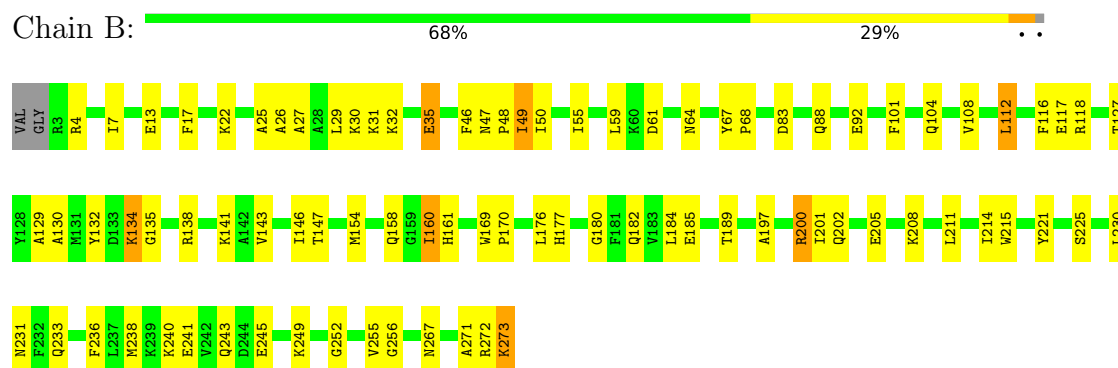
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

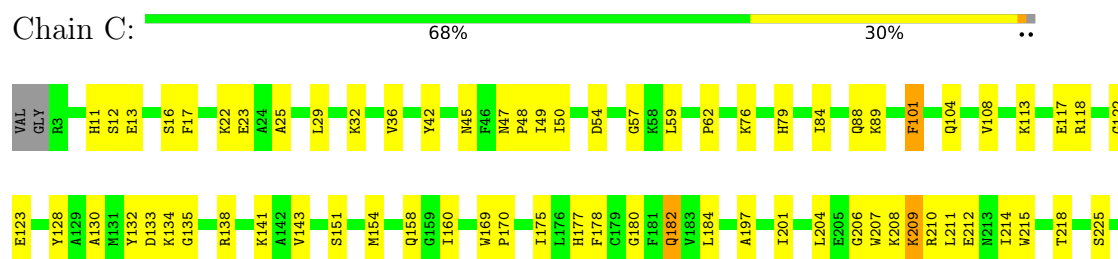
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1



• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

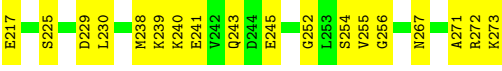
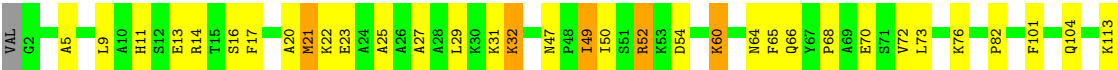


• Molecule 1: NAD(P)H dehydrogenase [quinone] 1





● Molecule 1: NAD(P)H dehydrogenase [quinone] 1



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.48Å 56.77Å 96.91Å 77.25° 76.83° 86.90°	Depositor
Resolution (Å)	32.19 – 1.80	Depositor
% Data completeness (in resolution range)	94.6 (32.19-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9494	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, 936

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	0.46	0/2226	0.97	12/3005 (0.4%)
1	B	0.46	0/2222	0.96	10/3000 (0.3%)
1	C	0.44	0/2222	0.92	7/3000 (0.2%)
1	D	0.47	0/2226	0.94	11/3005 (0.4%)
All	All	0.46	0/8896	0.95	40/12010 (0.3%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	182	GLN	N-CA-C	-8.91	94.66	109.46
1	A	182	GLN	N-CA-C	-8.55	95.27	109.46
1	C	182	GLN	N-CA-C	-8.47	95.49	108.96
1	B	182	GLN	N-CA-C	-7.43	97.15	108.96
1	B	49	ILE	N-CA-C	7.35	118.46	107.80
1	D	101	PHE	N-CA-C	7.29	114.78	108.22
1	C	101	PHE	N-CA-C	6.76	114.22	108.13
1	A	35	GLU	N-CA-C	-6.64	98.41	109.24
1	C	36	VAL	N-CA-C	6.41	117.14	108.17
1	B	35	GLU	N-CA-C	-6.16	98.69	108.73
1	A	232	PHE	N-CA-C	6.14	117.66	110.97
1	B	61	ASP	CA-C-N	6.09	125.81	119.05
1	B	61	ASP	C-N-CA	6.09	125.81	119.05
1	B	176	LEU	N-CA-C	6.08	117.60	110.97
1	A	49	ILE	N-CA-C	6.05	116.52	107.51
1	D	13	GLU	N-CA-C	6.04	118.58	108.73
1	B	13	GLU	N-CA-C	5.96	118.95	109.24
1	A	252	GLY	N-CA-C	-5.92	103.08	112.66
1	D	135	GLY	CA-C-N	5.83	127.12	119.84
1	D	135	GLY	C-N-CA	5.83	127.12	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ILE	CB-CA-C	-5.69	104.58	112.04
1	A	135	GLY	CA-C-N	5.63	125.47	119.28
1	A	135	GLY	C-N-CA	5.63	125.47	119.28
1	B	160	ILE	N-CA-C	5.59	117.00	110.62
1	C	13	GLU	N-CA-C	5.58	117.82	108.73
1	D	252	GLY	N-CA-C	-5.57	103.89	112.85
1	A	160	ILE	CB-CA-C	-5.41	104.96	112.04
1	A	95	ASP	N-CA-C	-5.36	105.55	112.68
1	D	195	THR	CA-C-N	5.36	125.35	119.89
1	D	195	THR	C-N-CA	5.36	125.35	119.89
1	D	146	ILE	N-CA-C	5.34	116.28	108.53
1	C	135	GLY	CA-C-N	5.34	125.01	119.56
1	C	135	GLY	C-N-CA	5.34	125.01	119.56
1	C	175	ILE	CB-CA-C	-5.28	107.22	111.71
1	D	49	ILE	N-CA-C	5.20	115.33	107.80
1	A	176	LEU	N-CA-C	5.16	116.75	111.03
1	A	218	THR	N-CA-C	-5.13	103.18	109.65
1	B	252	GLY	N-CA-C	-5.09	104.41	112.66
1	A	146	ILE	N-CA-C	5.07	115.89	108.53
1	D	163	ASP	N-CA-C	5.02	117.44	109.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2168	0	2167	73	0
1	B	2164	0	2164	79	0
1	C	2164	0	2164	67	0
1	D	2168	0	2167	83	0
2	A	53	0	31	6	0
2	B	53	0	31	3	0
2	C	53	0	31	3	0
2	D	53	0	31	3	0
3	A	26	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	16	2	0
3	C	26	0	16	2	0
3	D	26	0	16	3	0
4	A	129	0	0	5	0
4	B	144	0	0	6	0
4	C	114	0	0	3	0
4	D	127	0	0	5	0
All	All	9494	0	8850	290	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 16.

All (290) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:MET:HE3	1:D:204:LEU:HD23	1.29	1.11
1:B:108:VAL:CG2	1:B:112:LEU:HD13	1.94	0.97
1:B:160:ILE:HD12	1:D:131:MET:HE1	1.47	0.94
1:C:151:SER:H	1:C:154:MET:HE3	1.33	0.93
1:B:135:GLY:O	1:B:138:ARG:HG3	1.68	0.93
1:A:14:ARG:H	1:A:14:ARG:NE	1.68	0.92
1:D:17:PHE:HB2	2:D:604:FAD:H52A	1.51	0.92
1:A:50:ILE:HG13	1:A:118:ARG:HG2	1.53	0.90
1:A:14:ARG:H	1:A:14:ARG:HE	0.90	0.90
1:D:64:ASN:HD21	1:D:66:GLN:HE21	1.21	0.86
1:D:143:VAL:HG12	1:D:184:LEU:HB2	1.55	0.86
1:A:50:ILE:HD12	1:A:117:GLU:HB3	1.57	0.86
1:B:154:MET:HE3	1:B:160:ILE:HD11	1.59	0.84
1:A:17:PHE:HB2	2:A:601:FAD:H52A	1.60	0.83
1:D:143:VAL:CG1	1:D:184:LEU:HB2	2.08	0.83
1:B:108:VAL:HG21	1:B:112:LEU:HD13	1.61	0.82
1:A:108:VAL:CG1	1:A:112:LEU:HB3	2.11	0.81
1:B:238:MET:HE3	1:B:243:GLN:HG2	1.64	0.80
1:B:48:PRO:HG3	1:D:49:ILE:HD11	1.64	0.79
1:C:206:GLY:O	1:C:209:LYS:HD3	1.82	0.79
1:A:14:ARG:HE	1:A:14:ARG:N	1.75	0.78
1:B:17:PHE:HB2	2:B:602:FAD:H52A	1.65	0.77
1:C:50:ILE:HG22	1:C:118:ARG:HG2	1.66	0.77
1:D:64:ASN:HD21	1:D:66:GLN:NE2	1.83	0.77
1:D:60:LYS:HG3	1:D:70:GLU:OE1	1.84	0.76
1:D:238:MET:HE3	1:D:243:GLN:HG2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:VAL:HG22	1:B:184:LEU:HB2	1.68	0.74
1:C:17:PHE:HB2	2:C:603:FAD:H52A	1.69	0.73
1:A:127:THR:HG22	1:A:129:ALA:H	1.54	0.73
1:A:68:PRO:O	1:A:72:VAL:HG23	1.88	0.73
1:A:58:LYS:N	1:A:58:LYS:HD2	2.02	0.73
1:D:64:ASN:ND2	1:D:66:GLN:HE21	1.88	0.72
1:D:60:LYS:HG2	1:D:73:LEU:CD2	2.18	0.72
1:B:231:ASN:ND2	1:B:233:GLN:HB3	2.05	0.72
1:C:273:LYS:H	1:C:273:LYS:HD2	1.54	0.72
1:B:236:PHE:HB3	1:D:160:ILE:HG13	1.74	0.69
1:A:50:ILE:CD1	1:A:117:GLU:HB3	2.22	0.69
1:A:189:THR:HG22	4:A:777:HOH:O	1.92	0.69
1:A:148:THR:HG23	2:A:601:FAD:O2	1.93	0.69
1:B:231:ASN:HD21	1:B:233:GLN:HB3	1.58	0.69
1:A:273:LYS:HG2	1:A:273:LYS:OXT	1.91	0.68
1:D:189:THR:HG23	4:D:719:HOH:O	1.94	0.68
1:D:52:ARG:HG2	4:D:752:HOH:O	1.94	0.67
1:A:160:ILE:HG13	1:C:236:PHE:HB3	1.76	0.67
1:C:89:LYS:HG3	4:C:748:HOH:O	1.95	0.66
1:B:158:GLN:HB3	1:D:238:MET:HE2	1.76	0.66
1:D:169:TRP:CZ2	1:D:256:GLY:HA3	2.31	0.66
1:D:255:VAL:HG23	1:D:267:ASN:HD22	1.60	0.66
1:A:160:ILE:CG1	1:C:236:PHE:HB3	2.27	0.65
1:C:57:GLY:H	1:C:79:HIS:HB3	1.60	0.65
1:D:25:ALA:O	1:D:29:LEU:HD13	1.96	0.65
1:D:273:LYS:HB3	4:D:750:HOH:O	1.96	0.64
1:C:204:LEU:O	1:C:208:LYS:HG3	1.97	0.64
1:A:189:THR:HG23	4:A:773:HOH:O	1.98	0.64
1:C:59:LEU:HB2	1:C:62:PRO:HG3	1.80	0.63
1:C:243:GLN:O	1:C:247:LYS:HG3	1.98	0.63
1:A:200:ARG:NH1	2:A:601:FAD:H1B	2.13	0.63
1:D:189:THR:HG22	4:D:773:HOH:O	1.98	0.63
1:B:88:GLN:O	1:B:92:GLU:HG3	1.99	0.63
1:D:50:ILE:HG22	1:D:118:ARG:HG2	1.80	0.63
1:B:50:ILE:HG12	1:B:67:TYR:CZ	2.34	0.63
1:C:238:MET:HE3	1:C:243:GLN:HG2	1.80	0.63
1:D:60:LYS:HG2	1:D:73:LEU:HD22	1.80	0.62
1:B:50:ILE:HD12	1:B:117:GLU:HB3	1.80	0.62
1:A:108:VAL:HG11	1:A:112:LEU:HB3	1.81	0.62
1:B:160:ILE:HD12	1:D:131:MET:CE	2.26	0.62
1:B:25:ALA:O	1:B:29:LEU:HD13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:LYS:NZ	1:D:31:LYS:HB3	2.15	0.61
1:D:151:SER:H	1:D:154:MET:HE3	1.66	0.61
1:D:60:LYS:CD	1:D:73:LEU:HD22	2.31	0.60
1:B:112:LEU:HD22	1:B:116:PHE:CE2	2.37	0.60
1:B:134:LYS:HA	1:B:138:ARG:HD3	1.82	0.60
1:A:108:VAL:CG1	1:A:112:LEU:HD13	2.31	0.60
1:A:198:ASP:O	1:A:202:GLN:HG2	2.02	0.60
1:D:76:LYS:HE2	1:D:123:GLU:OE2	2.02	0.60
1:B:27:ALA:O	1:B:31:LYS:HG3	2.01	0.60
1:D:201:ILE:O	1:D:205:GLU:HG2	2.02	0.60
1:A:3:ARG:HB3	1:A:95:ASP:OD2	2.02	0.59
1:A:2:GLY:O	1:A:3:ARG:HB2	2.03	0.59
1:A:108:VAL:HG11	1:A:112:LEU:HD13	1.83	0.59
1:C:169:TRP:CZ2	1:C:256:GLY:HA3	2.38	0.59
1:A:270:LYS:HB2	1:A:272:ARG:NH1	2.18	0.59
1:A:50:ILE:HD11	1:A:117:GLU:O	2.03	0.58
1:B:134:LYS:HE3	1:B:225:SER:OG	2.03	0.58
1:D:138:ARG:HA	1:D:180:GLY:O	2.03	0.58
1:A:4:ARG:HD3	1:A:35:GLU:OE1	2.04	0.57
1:A:197:ALA:O	1:A:201:ILE:HG12	2.04	0.57
1:C:130:ALA:HB1	1:C:134:LYS:O	2.04	0.57
1:C:169:TRP:HB3	1:C:170:PRO:HD3	1.85	0.57
1:C:122:GLY:O	1:C:123:GLU:HB2	2.05	0.57
1:A:58:LYS:HD2	1:A:58:LYS:H	1.68	0.57
1:B:108:VAL:HG22	1:B:112:LEU:HB3	1.87	0.56
1:D:27:ALA:O	1:D:31:LYS:HG3	2.06	0.56
1:A:132:TYR:O	1:A:180:GLY:HA2	2.05	0.56
1:C:246:GLU:HG3	4:C:733:HOH:O	2.06	0.56
1:B:271:ALA:O	1:B:272:ARG:HB2	2.06	0.56
1:A:50:ILE:HG12	1:A:67:TYR:CZ	2.41	0.56
1:D:20:ALA:HA	1:D:23:GLU:OE2	2.05	0.56
1:B:4:ARG:HB3	4:B:796:HOH:O	2.06	0.56
1:B:50:ILE:HG13	1:B:118:ARG:HG2	1.87	0.55
1:D:122:GLY:O	1:D:123:GLU:HB2	2.05	0.55
1:D:169:TRP:HB3	1:D:170:PRO:HD3	1.88	0.55
1:D:197:ALA:O	1:D:201:ILE:HG13	2.06	0.55
1:B:169:TRP:HB3	1:B:170:PRO:HD3	1.86	0.55
1:D:131:MET:HE3	1:D:132:TYR:CD2	2.41	0.55
1:B:236:PHE:HD2	1:D:160:ILE:HD12	1.72	0.55
1:B:230:LEU:HD22	1:D:160:ILE:HD13	1.87	0.55
1:B:141:LYS:HD3	1:B:184:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:LEU:O	1:D:208:LYS:HG3	2.06	0.55
1:B:202:GLN:HA	1:B:202:GLN:NE2	2.21	0.54
1:B:154:MET:HE2	1:B:161:HIS:NE2	2.22	0.54
1:A:231:ASN:ND2	1:A:233:GLN:HE21	2.05	0.54
1:B:29:LEU:HD11	1:B:211:LEU:HB3	1.90	0.54
1:C:25:ALA:O	1:C:29:LEU:HD13	2.07	0.54
1:D:31:LYS:HB3	1:D:31:LYS:HZ3	1.71	0.54
1:A:138:ARG:HA	1:A:180:GLY:O	2.08	0.54
1:C:76:LYS:HE3	1:C:123:GLU:HG3	1.89	0.54
1:C:233:GLN:HA	1:C:233:GLN:HE21	1.72	0.54
1:A:2:GLY:O	1:A:3:ARG:CB	2.56	0.53
1:A:4:ARG:HD2	1:A:93:ALA:O	2.08	0.53
1:B:127:THR:HG22	1:B:129:ALA:H	1.74	0.53
1:B:169:TRP:CZ2	1:B:256:GLY:HA3	2.44	0.53
1:C:143:VAL:HG22	1:C:184:LEU:HB2	1.90	0.53
1:C:47:ASN:ND2	1:C:49:ILE:H	2.07	0.53
1:D:21:MET:HE3	1:D:204:LEU:CD2	2.20	0.53
4:B:837:HOH:O	1:D:52:ARG:HD3	2.08	0.53
1:B:143:VAL:CG2	1:B:184:LEU:HD12	2.39	0.52
1:B:132:TYR:O	1:B:180:GLY:HA2	2.09	0.52
1:B:238:MET:CE	1:B:243:GLN:HG2	2.37	0.52
1:B:4:ARG:HG2	1:B:35:GLU:OE1	2.09	0.52
1:D:17:PHE:HB2	2:D:604:FAD:C5B	2.33	0.52
1:D:23:GLU:HB3	4:D:784:HOH:O	2.10	0.52
1:A:200:ARG:HH11	2:A:601:FAD:H1B	1.74	0.52
1:B:134:LYS:HB2	1:B:134:LYS:NZ	2.25	0.52
1:A:91:LEU:HD11	1:A:120:PHE:HE1	1.75	0.51
1:D:60:LYS:CG	1:D:73:LEU:HD22	2.40	0.51
1:A:131:MET:HE3	1:C:160:ILE:HD13	1.91	0.51
1:D:76:LYS:CE	1:D:123:GLU:HG3	2.41	0.51
1:B:47:ASN:ND2	1:B:49:ILE:H	2.09	0.50
1:C:84:ILE:O	1:C:88:GLN:HG3	2.11	0.50
1:B:26:ALA:O	1:B:30:LYS:HG3	2.12	0.50
1:B:255:VAL:HG23	1:B:267:ASN:HD22	1.76	0.50
1:C:143:VAL:CG2	1:C:184:LEU:HD12	2.41	0.50
1:D:104:GLN:HA	2:D:604:FAD:C5X	2.42	0.50
1:B:46:PHE:O	1:B:48:PRO:HD3	2.12	0.50
1:A:108:VAL:HG12	1:A:112:LEU:HB3	1.92	0.49
1:A:270:LYS:HB3	1:A:272:ARG:HD3	1.94	0.49
1:D:131:MET:SD	3:D:702:936:H281	2.52	0.49
1:B:147:THR:HG22	1:B:189:THR:OG1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:TYR:O	1:C:180:GLY:HA2	2.12	0.49
1:A:154:MET:HE2	1:A:161:HIS:NE2	2.28	0.49
1:C:57:GLY:HA3	1:C:79:HIS:CG	2.47	0.49
1:A:169:TRP:CZ2	1:A:256:GLY:HA3	2.47	0.49
1:B:158:GLN:CB	1:D:238:MET:HE2	2.42	0.49
1:C:197:ALA:O	1:C:201:ILE:HG13	2.11	0.49
1:B:132:TYR:HA	1:B:177:HIS:O	2.13	0.49
1:A:4:ARG:HD3	1:A:35:GLU:CD	2.37	0.48
1:B:214:ILE:HG23	1:B:215:TRP:N	2.29	0.48
1:B:64:ASN:ND2	4:B:807:HOH:O	2.46	0.48
1:A:148:THR:HG22	1:A:150:GLY:N	2.29	0.48
1:D:20:ALA:HA	1:D:23:GLU:HG2	1.95	0.48
1:D:214:ILE:HD12	1:D:217:GLU:OE2	2.14	0.48
1:B:185:GLU:HG3	4:B:714:HOH:O	2.13	0.48
1:C:242:VAL:O	1:C:246:GLU:HB2	2.14	0.48
1:C:113:LYS:O	1:C:117:GLU:HG3	2.13	0.48
1:B:230:LEU:HD22	1:D:160:ILE:CD1	2.43	0.48
3:C:701:936:H291	3:C:701:936:H192	1.68	0.48
1:A:50:ILE:HD11	1:A:117:GLU:C	2.39	0.47
1:B:55:ILE:HG21	1:B:59:LEU:HD23	1.95	0.47
1:B:104:GLN:HA	2:B:602:FAD:C5X	2.44	0.47
1:B:189:THR:HG23	4:B:712:HOH:O	2.13	0.47
1:C:76:LYS:CE	1:C:123:GLU:HG3	2.45	0.47
1:C:132:TYR:CD1	1:C:178:PHE:HA	2.49	0.47
1:A:132:TYR:HA	1:A:177:HIS:O	2.14	0.47
1:A:47:ASN:ND2	1:A:49:ILE:H	2.11	0.47
1:C:141:LYS:HE2	1:C:182:GLN:OE1	2.14	0.47
1:A:192:ILE:CG2	2:A:601:FAD:H5'1	2.45	0.47
1:C:132:TYR:HA	1:C:177:HIS:O	2.14	0.47
1:A:52:ARG:HG2	4:A:719:HOH:O	2.14	0.47
1:D:9:LEU:HD22	1:D:22:LYS:HD3	1.96	0.47
1:B:236:PHE:HD2	1:D:160:ILE:CD1	2.27	0.46
1:D:241:GLU:O	1:D:245:GLU:HG3	2.15	0.46
1:A:231:ASN:HD21	1:A:233:GLN:HE21	1.63	0.46
1:B:154:MET:HE2	1:B:161:HIS:CD2	2.50	0.46
1:D:128:TYR:HB3	3:D:702:936:O35	2.14	0.46
1:A:73:LEU:HD23	4:A:780:HOH:O	2.16	0.46
1:C:238:MET:HE2	1:C:259:LEU:HD21	1.98	0.46
1:D:255:VAL:H	1:D:267:ASN:ND2	2.14	0.46
1:D:254:SER:HB2	1:D:267:ASN:HD21	1.80	0.46
1:A:253:LEU:HD22	4:A:793:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:TYR:HB3	1:B:68:PRO:HD3	1.98	0.46
1:C:207:TRP:HZ3	1:C:210:ARG:HD3	1.80	0.46
1:C:104:GLN:HA	2:C:603:FAD:C5X	2.46	0.46
1:C:12:SER:HB3	1:C:42:TYR:CE1	2.51	0.46
1:A:231:ASN:HD21	1:A:233:GLN:NE2	2.14	0.45
3:D:702:936:H291	3:D:702:936:H192	1.56	0.45
1:C:29:LEU:CD1	1:C:211:LEU:HD13	2.46	0.45
1:A:195:THR:HG22	1:A:199:ALA:HB3	1.98	0.45
1:B:31:LYS:NZ	1:B:208:LYS:NZ	2.64	0.45
1:A:130:ALA:HB1	1:A:134:LYS:O	2.16	0.45
1:C:133:ASP:CG	1:C:225:SER:H	2.25	0.45
1:C:218:THR:HG23	1:C:271:ALA:HB3	1.97	0.45
1:B:29:LEU:CD1	1:B:211:LEU:HB3	2.47	0.45
1:B:32:LYS:HD2	4:B:785:HOH:O	2.17	0.45
1:B:108:VAL:CG2	1:B:112:LEU:CD1	2.81	0.45
1:B:197:ALA:HA	1:B:200:ARG:NH1	2.32	0.45
1:C:255:VAL:HG23	1:C:267:ASN:HD22	1.82	0.45
1:B:83:ASP:OD2	1:B:118:ARG:NH2	2.33	0.45
1:C:23:GLU:OE1	1:C:23:GLU:HA	2.16	0.45
1:C:45:ASN:HB3	4:C:772:HOH:O	2.16	0.45
1:D:132:TYR:O	1:D:180:GLY:HA2	2.16	0.45
1:A:108:VAL:O	1:C:113:LYS:NZ	2.50	0.45
1:C:273:LYS:HZ2	1:C:273:LYS:N	2.15	0.45
1:D:60:LYS:HG2	1:D:73:LEU:HD23	1.93	0.45
1:A:67:TYR:HB3	1:A:68:PRO:HD3	1.99	0.44
1:B:135:GLY:O	1:B:138:ARG:NH1	2.49	0.44
1:C:50:ILE:CG2	1:C:118:ARG:HG2	2.44	0.44
1:A:122:GLY:O	1:A:123:GLU:HB3	2.17	0.44
1:B:4:ARG:HG2	1:B:35:GLU:CD	2.42	0.44
1:B:108:VAL:HG23	1:B:112:LEU:HD13	1.94	0.44
3:B:704:936:H291	3:B:704:936:H192	1.80	0.44
1:C:32:LYS:HD2	1:C:212:GLU:HG2	1.98	0.44
1:C:239:LYS:HB2	1:C:242:VAL:HG23	1.99	0.44
1:D:132:TYR:HA	1:D:177:HIS:O	2.18	0.44
1:D:52:ARG:HG2	1:D:52:ARG:H	1.53	0.44
1:C:231:ASN:OD1	1:C:233:GLN:HB3	2.17	0.44
1:C:273:LYS:H	1:C:273:LYS:CD	2.27	0.44
1:D:60:LYS:HD3	1:D:73:LEU:HD22	1.99	0.43
1:D:211:LEU:HA	1:D:214:ILE:HB	2.01	0.43
1:A:108:VAL:HG23	1:A:171:ILE:HD13	2.00	0.43
1:B:201:ILE:O	1:B:205:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ASP:CG	1:C:118:ARG:HD2	2.43	0.43
1:A:77:GLU:HB2	1:A:79:HIS:CE1	2.54	0.43
1:D:76:LYS:HE2	1:D:123:GLU:HG3	1.99	0.43
1:D:113:LYS:O	1:D:117:GLU:HG3	2.19	0.43
1:D:131:MET:HE3	1:D:132:TYR:CE2	2.54	0.43
1:D:11:HIS:CE1	1:D:16:SER:HB3	2.54	0.43
1:D:47:ASN:ND2	1:D:49:ILE:H	2.16	0.43
1:A:73:LEU:O	1:A:77:GLU:HG3	2.19	0.43
3:B:704:936:H251	1:D:150:GLY:HA2	2.01	0.43
1:D:271:ALA:O	1:D:272:ARG:HB2	2.19	0.43
1:A:80:LEU:O	1:A:81:SER:C	2.62	0.43
1:C:233:GLN:HE21	1:C:233:GLN:CA	2.31	0.43
1:D:65:PHE:CE2	1:D:70:GLU:HG3	2.53	0.42
1:C:22:LYS:HE3	1:C:23:GLU:OE1	2.19	0.42
1:A:219:PRO:C	1:A:271:ALA:HB1	2.44	0.42
1:B:127:THR:HB	1:B:130:ALA:HB3	2.01	0.42
1:D:32:LYS:HB3	1:D:32:LYS:NZ	2.34	0.42
1:C:17:PHE:HB2	2:C:603:FAD:C5B	2.46	0.42
1:D:5:ALA:CB	1:D:29:LEU:HD23	2.50	0.42
1:D:29:LEU:CD1	1:D:211:LEU:HD13	2.49	0.42
1:A:31:LYS:HB2	1:A:31:LYS:HE3	1.79	0.42
1:A:238:MET:CE	1:A:242:VAL:HG12	2.49	0.42
1:B:230:LEU:CD2	1:D:160:ILE:HD13	2.50	0.42
1:D:151:SER:OG	1:D:154:MET:HE3	2.19	0.42
1:A:148:THR:CG2	1:A:149:GLY:N	2.82	0.42
1:B:31:LYS:HZ2	1:B:208:LYS:NZ	2.18	0.42
1:C:206:GLY:HA2	1:C:209:LYS:HD2	2.02	0.42
1:A:17:PHE:HB2	2:A:601:FAD:C5B	2.42	0.41
3:A:703:936:H192	3:A:703:936:H291	1.75	0.41
1:B:29:LEU:CD1	1:B:211:LEU:HD13	2.50	0.41
1:B:221:TYR:HB2	1:B:273:LYS:HA	2.01	0.41
1:C:233:GLN:HA	1:C:233:GLN:NE2	2.33	0.41
1:B:272:ARG:O	1:B:273:LYS:HB2	2.19	0.41
1:C:141:LYS:NZ	1:C:215:TRP:O	2.51	0.41
1:D:229:ASP:OD1	1:D:239:LYS:HG2	2.20	0.41
1:C:138:ARG:HA	1:C:180:GLY:O	2.19	0.41
1:C:143:VAL:HG22	1:C:184:LEU:HD12	2.01	0.41
1:D:54:ASP:OD2	1:D:118:ARG:HD2	2.20	0.41
1:A:54:ASP:OD1	1:A:118:ARG:NH1	2.47	0.41
1:C:255:VAL:H	1:C:267:ASN:ND2	2.19	0.41
1:A:108:VAL:HG13	1:A:109:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLU:HG3	1:A:124:PHE:HE1	1.86	0.41
1:A:167:ILE:O	1:A:170:PRO:HD2	2.21	0.41
1:B:154:MET:CE	1:B:161:HIS:NE2	2.83	0.41
1:B:245:GLU:O	1:B:249:LYS:HE3	2.20	0.41
1:A:112:LEU:HD22	1:A:116:PHE:CE2	2.56	0.41
1:C:101:PHE:CZ	1:C:108:VAL:HG12	2.56	0.41
1:B:104:GLN:HA	2:B:602:FAD:N5	2.35	0.40
1:B:236:PHE:O	1:D:160:ILE:HG13	2.22	0.40
1:D:225:SER:HB2	1:D:230:LEU:HD11	2.02	0.40
1:A:214:ILE:HG23	1:A:215:TRP:N	2.36	0.40
1:B:7:ILE:HG21	1:B:22:LYS:HG2	2.02	0.40
1:B:101:PHE:CZ	1:B:146:ILE:HG12	2.56	0.40
1:C:11:HIS:CE1	1:C:16:SER:HB3	2.56	0.40
1:C:54:ASP:OD2	1:C:118:ARG:HD2	2.21	0.40
1:C:128:TYR:HB3	3:C:701:936:N34	2.36	0.40
1:D:68:PRO:O	1:D:72:VAL:HG23	2.22	0.40
1:C:211:LEU:HA	1:C:214:ILE:HB	2.02	0.40
1:D:240:LYS:HD2	1:D:240:LYS:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	134/227 (59%)	128 (96%)	6 (4%)	24	12
1	C	220/227 (97%)	215 (98%)	5 (2%)	44	33
1	D	226/227 (100%)	217 (96%)	9 (4%)	28	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	580/681 (85%)	560 (97%)	20 (3%)	32	20

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	112	LEU
1	B	134	LYS
1	B	200	ARG
1	B	240	LYS
1	B	241	GLU
1	B	273	LYS
1	C	48	PRO
1	C	158	GLN
1	C	209	LYS
1	C	241	GLU
1	C	273	LYS
1	D	14	ARG
1	D	21	MET
1	D	32	LYS
1	D	52	ARG
1	D	60	LYS
1	D	82	PRO
1	D	158	GLN
1	D	189	THR
1	D	202	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	267	ASN
1	B	268	GLN
1	C	47	ASN
1	C	104	GLN
1	C	158	GLN
1	C	172	GLN
1	C	233	GLN
1	C	267	ASN
1	C	268	GLN
1	D	47	ASN
1	D	66	GLN
1	D	79	HIS

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Mol	Chain	Res	Type
1	D	104	GLN
1	D	158	GLN
1	D	172	GLN
1	D	233	GLN
1	D	243	GLN
1	D	267	ASN
1	D	268	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	936	A	703	-	27,28,28	2.49	9 (33%)	30,41,41	1.19	2 (6%)
3	936	D	702	-	27,28,28	2.59	6 (22%)	30,41,41	1.30	3 (10%)
2	FAD	D	604	-	58,58,58	2.60	21 (36%)	85,89,89	1.12	6 (7%)
2	FAD	C	603	-	58,58,58	2.66	21 (36%)	85,89,89	1.14	6 (7%)
3	936	B	704	-	27,28,28	2.59	9 (33%)	30,41,41	1.18	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	601	-	58,58,58	2.71	19 (32%)	85,89,89	1.15	6 (7%)
2	FAD	B	602	-	58,58,58	2.69	18 (31%)	85,89,89	1.14	6 (7%)
3	936	C	701	-	27,28,28	2.48	6 (22%)	30,41,41	1.19	3 (10%)

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	936	A	703	-	-	5/9/27/27	0/3/3/3
3	936	D	702	-	-	5/9/27/27	0/3/3/3
2	FAD	D	604	-	-	5/34/50/50	0/6/6/6
2	FAD	C	603	-	-	6/34/50/50	0/6/6/6
3	936	B	704	-	-	5/9/27/27	0/3/3/3
2	FAD	A	601	-	-	5/34/50/50	0/6/6/6
2	FAD	B	602	-	-	4/34/50/50	0/6/6/6
3	936	C	701	-	-	5/9/27/27	0/3/3/3

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	FAD	P-O3P	-14.53	1.43	1.59
2	A	601	FAD	P-O3P	-14.35	1.44	1.59
2	C	603	FAD	P-O3P	-13.76	1.44	1.59
2	D	604	FAD	P-O3P	-13.21	1.45	1.59
3	D	702	936	O36-N34	10.78	1.41	1.22
3	B	704	936	O36-N34	10.43	1.40	1.22
3	C	701	936	O36-N34	10.08	1.40	1.22
3	A	703	936	O36-N34	9.62	1.39	1.22
2	A	601	FAD	C9A-N10	4.59	1.49	1.41
2	B	602	FAD	PA-O2A	-4.50	1.34	1.55
2	C	603	FAD	C9A-N10	4.37	1.48	1.41
2	A	601	FAD	PA-O2A	-4.32	1.35	1.55
2	C	603	FAD	PA-O2A	-4.28	1.35	1.55
2	D	604	FAD	C9A-N10	4.28	1.48	1.41
2	D	604	FAD	PA-O2A	-4.23	1.35	1.55
2	B	602	FAD	C9A-N10	4.04	1.48	1.41
3	A	703	936	C27-N34	-4.00	1.35	1.45
3	D	702	936	C27-N34	-3.90	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	604	FAD	C5A-C6A	3.63	1.51	1.41
2	B	602	FAD	PA-O5B	-3.63	1.45	1.59
2	A	601	FAD	C5A-C6A	3.62	1.51	1.41
3	C	701	936	C27-N34	-3.60	1.36	1.45
2	C	603	FAD	C5A-C6A	3.57	1.50	1.41
2	A	601	FAD	PA-O5B	-3.50	1.45	1.59
2	B	602	FAD	P-O2P	-3.48	1.39	1.55
2	B	602	FAD	C5A-C6A	3.46	1.50	1.41
3	B	704	936	C27-N34	-3.43	1.37	1.45
2	C	603	FAD	C4X-N5	3.40	1.38	1.30
2	C	603	FAD	C4A-N3A	3.40	1.40	1.34
2	B	602	FAD	C6-C5X	3.35	1.45	1.40
2	A	601	FAD	P-O2P	-3.34	1.39	1.55
2	D	604	FAD	C5A-C4A	3.30	1.45	1.39
2	D	604	FAD	P-O2P	-3.29	1.40	1.55
2	C	603	FAD	P-O2P	-3.25	1.40	1.55
2	B	602	FAD	C4X-N5	3.23	1.37	1.30
2	A	601	FAD	C4A-N3A	3.22	1.40	1.34
2	D	604	FAD	O5'-C5'	3.16	1.56	1.44
2	C	603	FAD	C5A-C4A	3.14	1.44	1.39
2	C	603	FAD	C8-C7	3.12	1.48	1.40
2	C	603	FAD	O5'-C5'	3.11	1.56	1.44
2	A	601	FAD	C4X-N5	3.11	1.37	1.30
2	D	604	FAD	C4A-N3A	3.08	1.40	1.34
2	A	601	FAD	O5'-C5'	3.06	1.56	1.44
2	D	604	FAD	C4X-N5	3.04	1.37	1.30
2	A	601	FAD	C6-C5X	3.04	1.44	1.40
2	D	604	FAD	PA-O5B	-3.03	1.47	1.59
2	A	601	FAD	C5A-C4A	3.03	1.44	1.39
2	B	602	FAD	C8-C7	3.02	1.48	1.40
3	B	704	936	C4-C5	-2.98	1.36	1.46
2	C	603	FAD	PA-O5B	-2.97	1.47	1.59
2	B	602	FAD	C2A-N1A	2.95	1.39	1.33
2	C	603	FAD	C9A-C5X	2.95	1.45	1.41
2	C	603	FAD	C2A-N1A	2.92	1.39	1.33
2	B	602	FAD	C5A-C4A	2.92	1.44	1.39
3	C	701	936	C4-C5	-2.91	1.37	1.46
2	A	601	FAD	C9A-C5X	2.91	1.45	1.41
2	A	601	FAD	C8-C7	2.89	1.47	1.40
2	D	604	FAD	C9A-C5X	2.88	1.45	1.41
2	D	604	FAD	O4B-C1B	2.88	1.48	1.42
2	D	604	FAD	C8-C7	2.88	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	604	FAD	C6-C5X	2.87	1.44	1.40
2	C	603	FAD	C2-N3	2.86	1.45	1.39
2	A	601	FAD	C9-C9A	2.84	1.44	1.39
3	D	702	936	C4-C5	-2.84	1.37	1.46
3	A	703	936	C4-C5	-2.82	1.37	1.46
2	B	602	FAD	O5'-C5'	2.82	1.55	1.44
3	A	703	936	C19-C9	2.80	1.56	1.50
2	A	601	FAD	C2A-N1A	2.78	1.38	1.33
2	B	602	FAD	C4A-N3A	2.77	1.39	1.34
2	D	604	FAD	C2A-N1A	2.71	1.38	1.33
2	C	603	FAD	C6-C5X	2.70	1.44	1.40
3	D	702	936	C29-C24	2.70	1.43	1.38
2	C	603	FAD	C9-C9A	2.66	1.43	1.39
2	D	604	FAD	C10-N1	2.64	1.38	1.33
2	B	602	FAD	C9A-C5X	2.62	1.45	1.41
2	A	601	FAD	O4B-C1B	2.62	1.48	1.42
2	B	602	FAD	C10-N1	2.62	1.38	1.33
3	B	704	936	C19-C9	2.54	1.56	1.50
3	C	701	936	C19-C9	2.52	1.56	1.50
2	A	601	FAD	C10-N1	2.51	1.38	1.33
2	C	603	FAD	O4B-C4B	2.47	1.50	1.45
3	B	704	936	O20-C24	2.46	1.43	1.37
2	D	604	FAD	C9-C9A	2.46	1.43	1.39
3	A	703	936	O20-C24	2.43	1.43	1.37
2	A	601	FAD	C9-C8	2.42	1.42	1.39
3	B	704	936	C29-C24	2.40	1.43	1.38
2	C	603	FAD	O4B-C1B	2.40	1.47	1.42
2	D	604	FAD	O4B-C4B	2.39	1.50	1.45
2	C	603	FAD	C10-N1	2.38	1.38	1.33
2	D	604	FAD	C2-N3	2.37	1.44	1.39
2	B	602	FAD	O4B-C1B	2.36	1.47	1.42
2	D	604	FAD	O2-C2	-2.32	1.19	1.24
3	C	701	936	C29-C24	2.31	1.43	1.38
2	B	602	FAD	C2-N3	2.30	1.44	1.39
3	B	704	936	C28-C27	2.27	1.43	1.38
2	D	604	FAD	C1'-C2'	2.25	1.55	1.52
2	B	602	FAD	C9-C9A	2.23	1.43	1.39
2	A	601	FAD	C2-N3	2.20	1.43	1.39
3	C	701	936	O20-C24	2.20	1.42	1.37
3	A	703	936	C29-C24	2.20	1.42	1.38
3	D	702	936	O20-C24	2.14	1.42	1.37
3	B	704	936	C25-C24	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	704	936	C29-C28	2.09	1.42	1.38
3	D	702	936	C37-C8	2.09	1.52	1.49
3	A	703	936	C25-C24	2.08	1.42	1.38
2	C	603	FAD	O2-C2	-2.07	1.20	1.24
3	A	703	936	O44-C6	2.05	1.40	1.36
2	C	603	FAD	C9-C8	2.04	1.42	1.39
3	A	703	936	C37-C8	2.02	1.52	1.49

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	936	O36-N34-C27	3.80	124.05	118.82
3	C	701	936	O36-N34-C27	3.53	123.68	118.82
3	D	702	936	C19-O20-C24	-3.46	111.44	117.63
3	B	704	936	O36-N34-C27	3.38	123.47	118.82
3	D	702	936	O36-N34-C27	3.26	123.30	118.82
2	D	604	FAD	O5B-PA-O1A	-3.14	96.50	108.94
2	C	603	FAD	O5B-PA-O1A	-3.03	96.93	108.94
2	C	603	FAD	C4'-C3'-C2'	-3.02	108.55	113.57
2	A	601	FAD	O5B-PA-O1A	-2.97	97.15	108.94
2	B	602	FAD	C4'-C3'-C2'	-2.94	108.68	113.57
2	A	601	FAD	C4'-C3'-C2'	-2.94	108.68	113.57
2	B	602	FAD	O5B-PA-O1A	-2.89	97.47	108.94
2	B	602	FAD	O2A-PA-O3P	2.76	114.72	107.27
2	A	601	FAD	O2A-PA-O3P	2.62	114.35	107.27
2	C	603	FAD	C5X-C9A-N10	-2.47	115.73	117.97
2	A	601	FAD	C5X-C9A-N10	-2.46	115.75	117.97
2	D	604	FAD	C2A-N1A-C6A	2.40	122.67	118.73
3	D	702	936	O44-C6-C5	2.38	118.42	112.14
2	D	604	FAD	C4'-C3'-C2'	-2.37	109.62	113.57
2	D	604	FAD	O2A-PA-O3P	2.34	113.60	107.27
2	C	603	FAD	C2A-N1A-C6A	2.31	122.53	118.73
2	D	604	FAD	C4-N3-C2	-2.27	121.61	125.64
2	D	604	FAD	C5X-C9A-N10	-2.26	115.92	117.97
2	B	602	FAD	C5X-C9A-N10	-2.25	115.93	117.97
2	A	601	FAD	C2A-N1A-C6A	2.25	122.42	118.73
2	C	603	FAD	C4-N3-C2	-2.25	121.66	125.64
3	C	701	936	C19-O20-C24	-2.23	113.64	117.63
3	B	704	936	O44-C6-C5	2.14	117.77	112.14
2	A	601	FAD	C4-N3-C2	-2.10	121.91	125.64
2	B	602	FAD	C2A-N1A-C6A	2.10	122.18	118.73
2	C	603	FAD	O2A-PA-O3P	2.09	112.92	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	FAD	C4-N3-C2	-2.08	121.94	125.64
3	C	701	936	O44-C6-C5	2.02	117.47	112.14
3	A	703	936	O44-C6-C5	2.01	117.43	112.14

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	936	O20-C19-C9-C4
3	A	703	936	O20-C19-C9-C8
3	A	703	936	C26-C27-N34-O36
3	A	703	936	C28-C27-N34-O36
3	B	704	936	O20-C19-C9-C4
3	B	704	936	O20-C19-C9-C8
3	C	701	936	O20-C19-C9-C4
3	C	701	936	O20-C19-C9-C8
3	D	702	936	O20-C19-C9-C4
3	D	702	936	O20-C19-C9-C8
3	D	702	936	C26-C27-N34-O36
3	D	702	936	C28-C27-N34-O36
3	C	701	936	C28-C27-N34-O36
3	A	703	936	C9-C19-O20-C24
3	B	704	936	C9-C19-O20-C24
3	C	701	936	C9-C19-O20-C24
3	D	702	936	C9-C19-O20-C24
3	B	704	936	C28-C27-N34-O36
3	C	701	936	C26-C27-N34-O36
2	A	601	FAD	C2B-C1B-N9A-C8A
2	B	602	FAD	C2B-C1B-N9A-C8A
2	C	603	FAD	C2B-C1B-N9A-C8A
2	D	604	FAD	C2B-C1B-N9A-C8A
2	B	602	FAD	PA-O3P-P-O2P
2	C	603	FAD	PA-O3P-P-O2P
2	D	604	FAD	PA-O3P-P-O2P
3	B	704	936	C26-C27-N34-O36
2	A	601	FAD	PA-O3P-P-O2P
2	C	603	FAD	C2B-C1B-N9A-C4A
2	D	604	FAD	C2B-C1B-N9A-C4A
2	A	601	FAD	C2B-C1B-N9A-C4A
2	A	601	FAD	O4B-C1B-N9A-C8A
2	C	603	FAD	O4B-C1B-N9A-C8A
2	C	603	FAD	PA-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
2	D	604	FAD	O4B-C1B-N9A-C8A
2	B	602	FAD	O4B-C1B-N9A-C8A
2	B	602	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	O4B-C4B-C5B-O5B
2	C	603	FAD	O4B-C4B-C5B-O5B
2	D	604	FAD	O4B-C4B-C5B-O5B

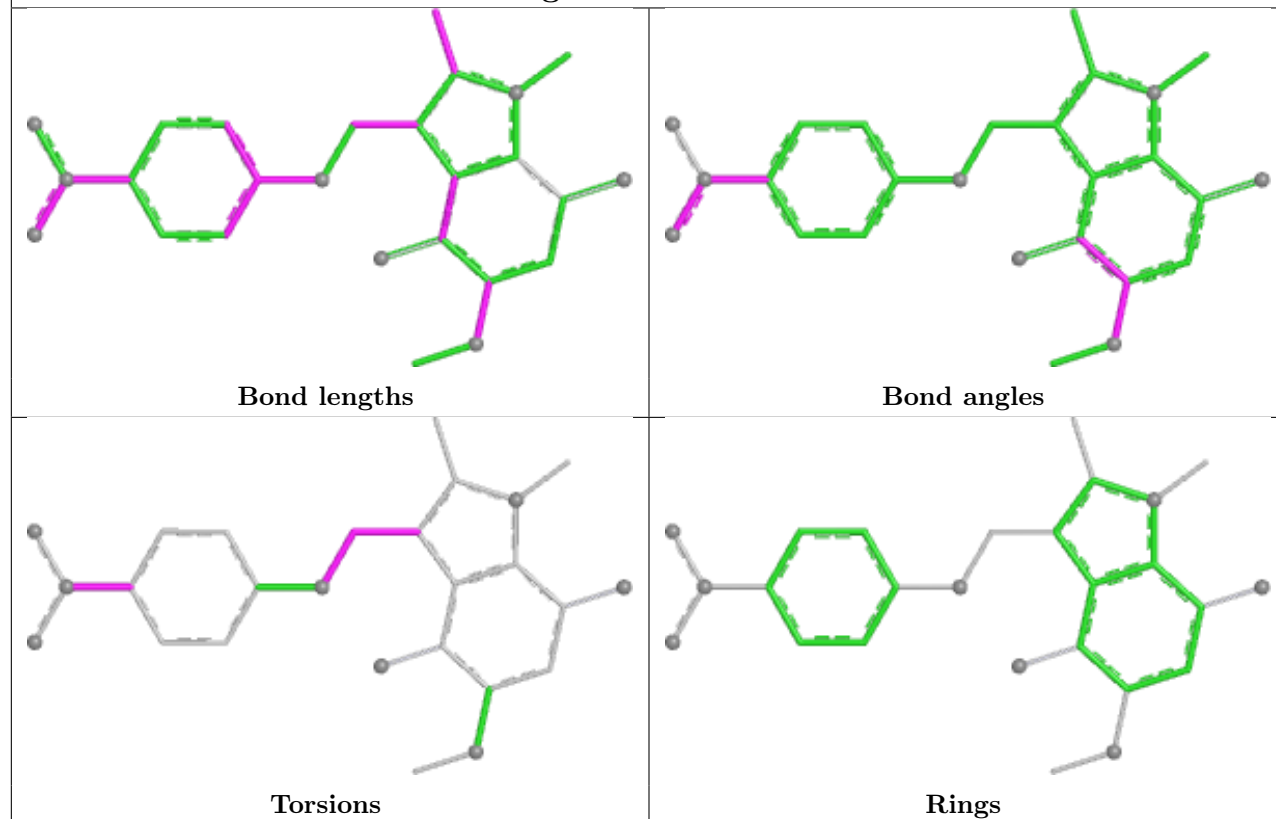
There are no ring outliers.

8 monomers are involved in 23 short contacts:

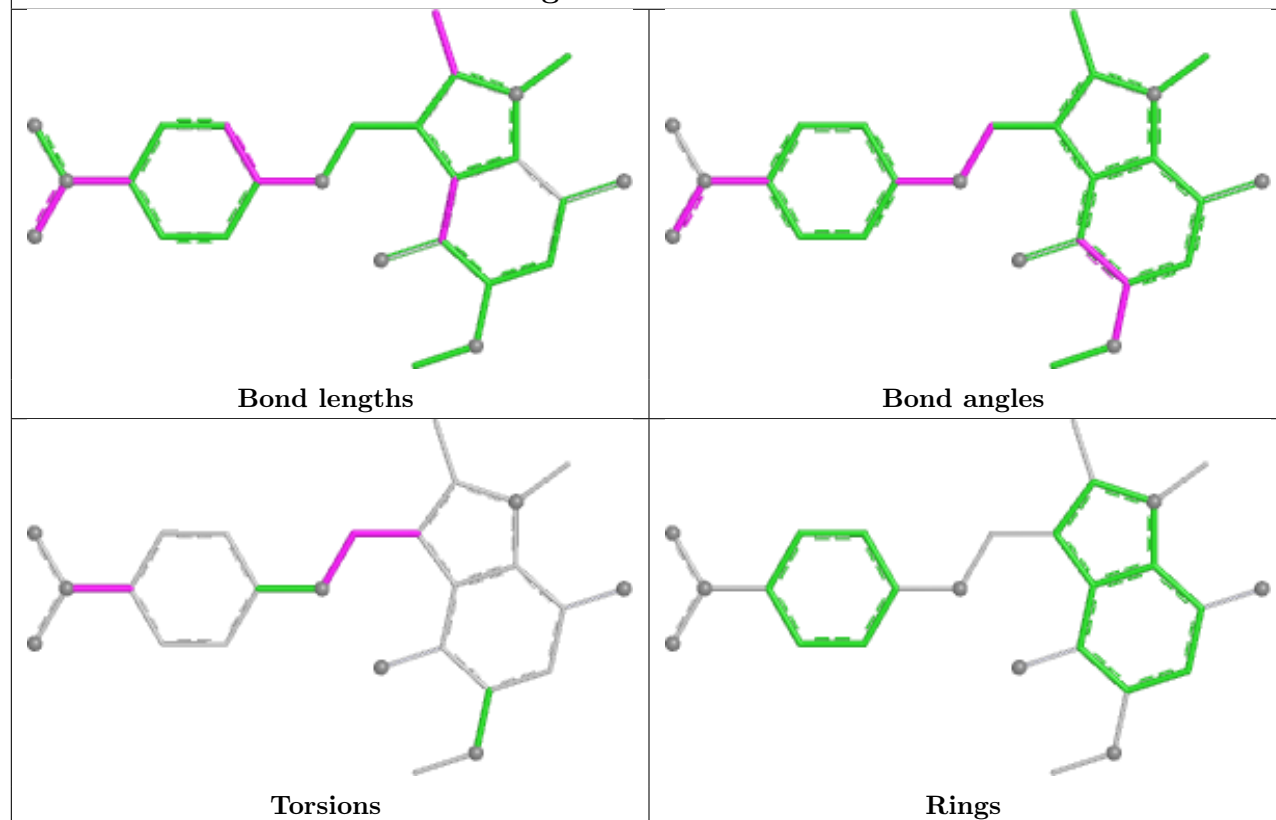
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	936	1	0
3	D	702	936	3	0
2	D	604	FAD	3	0
2	C	603	FAD	3	0
3	B	704	936	2	0
2	A	601	FAD	6	0
2	B	602	FAD	3	0
3	C	701	936	2	0

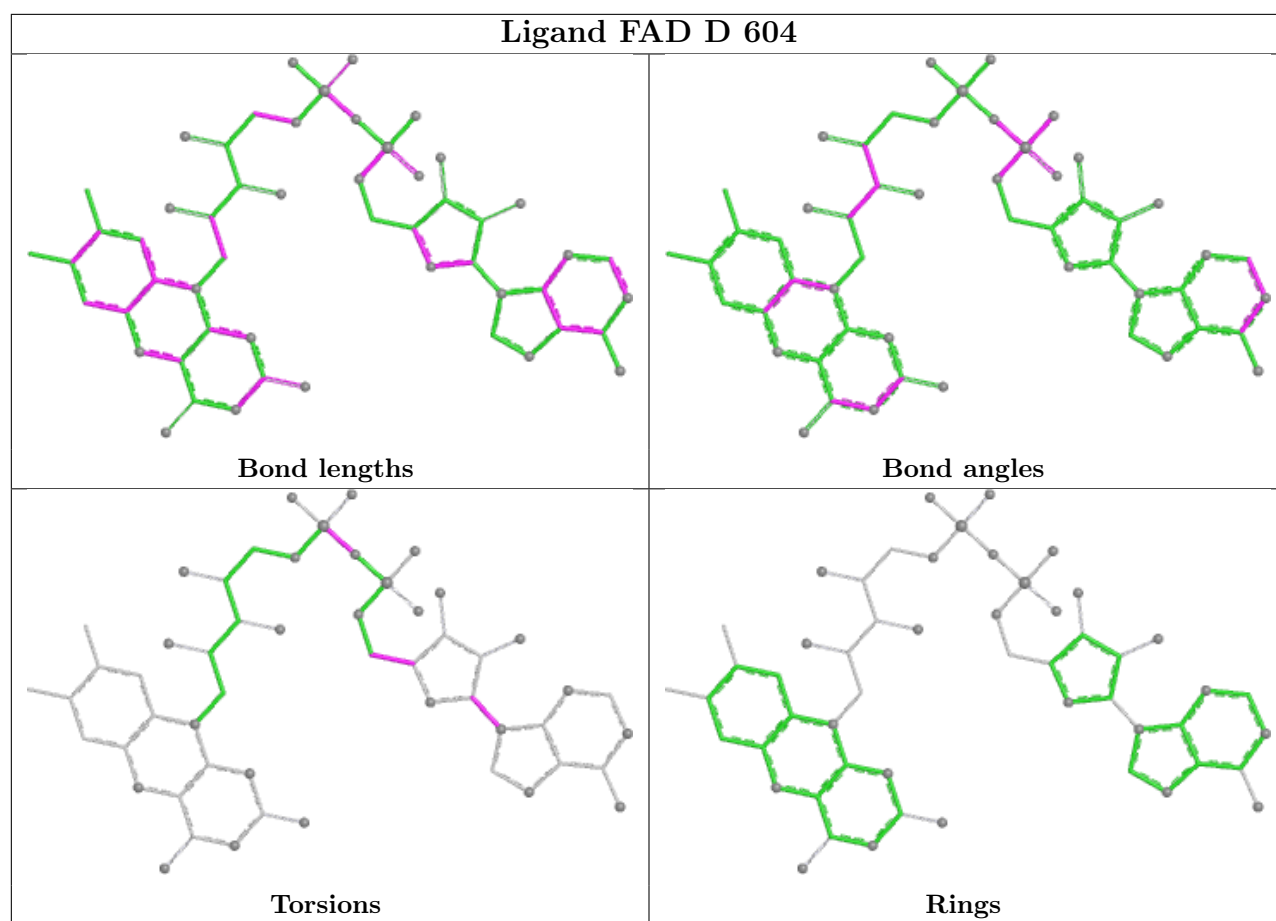
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 936 A 703

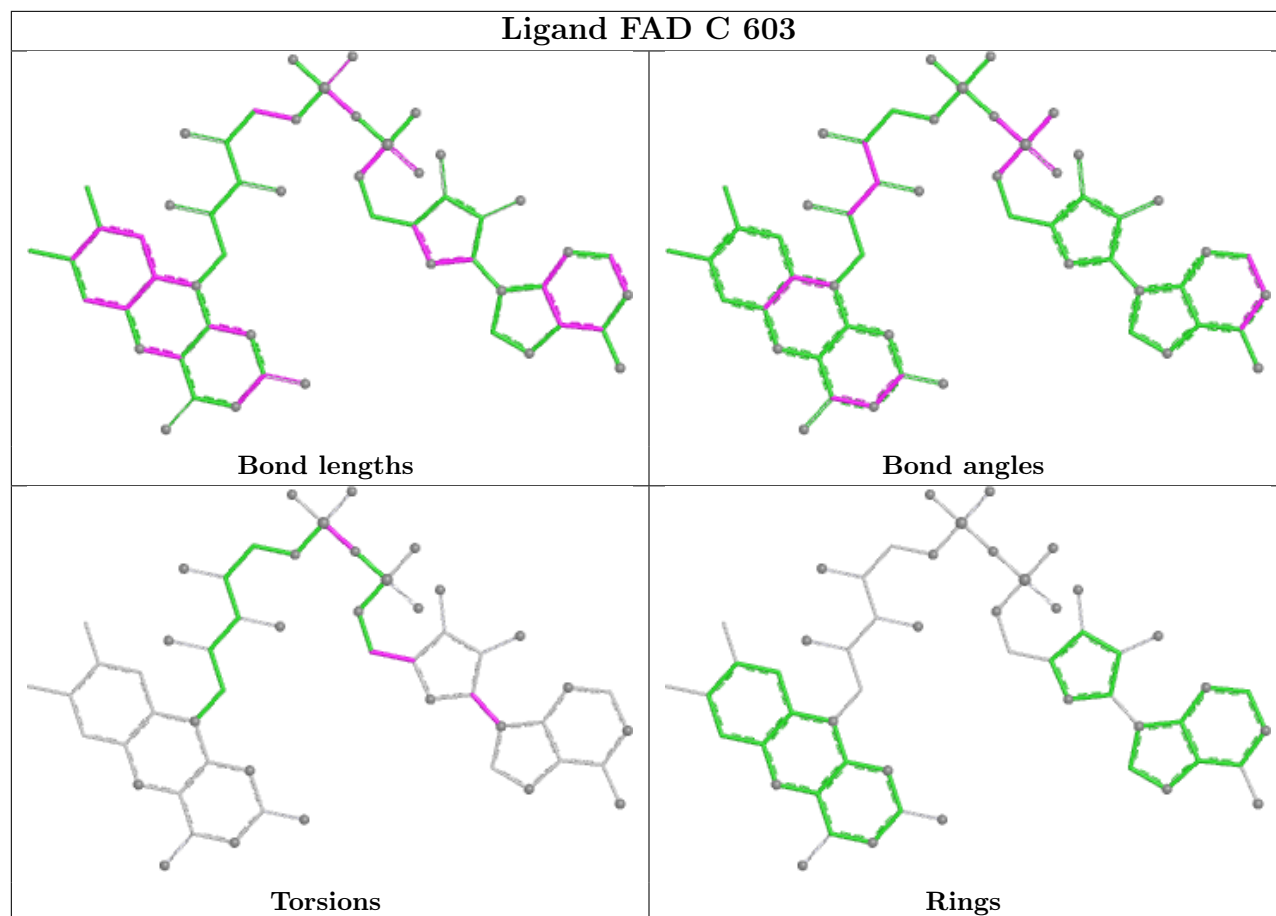


Ligand 936 D 702

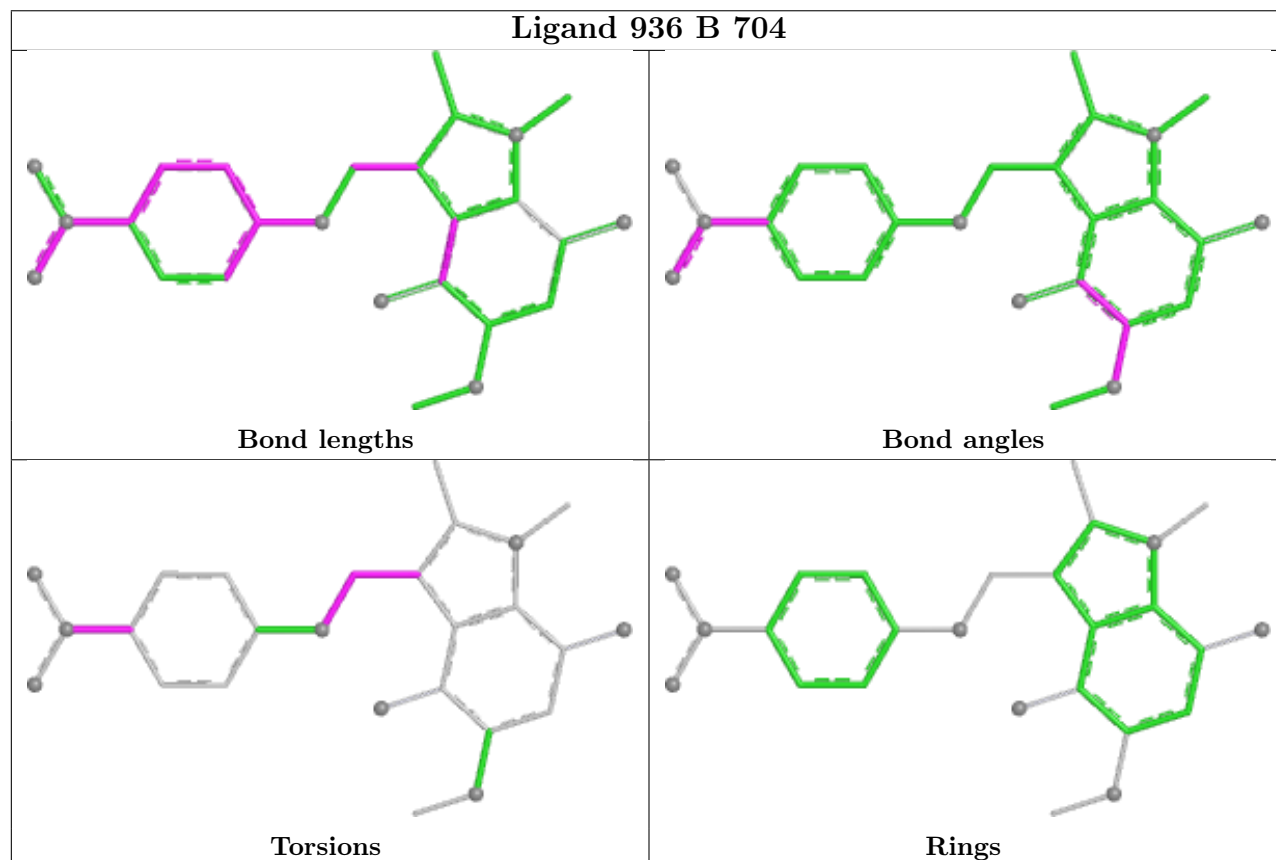




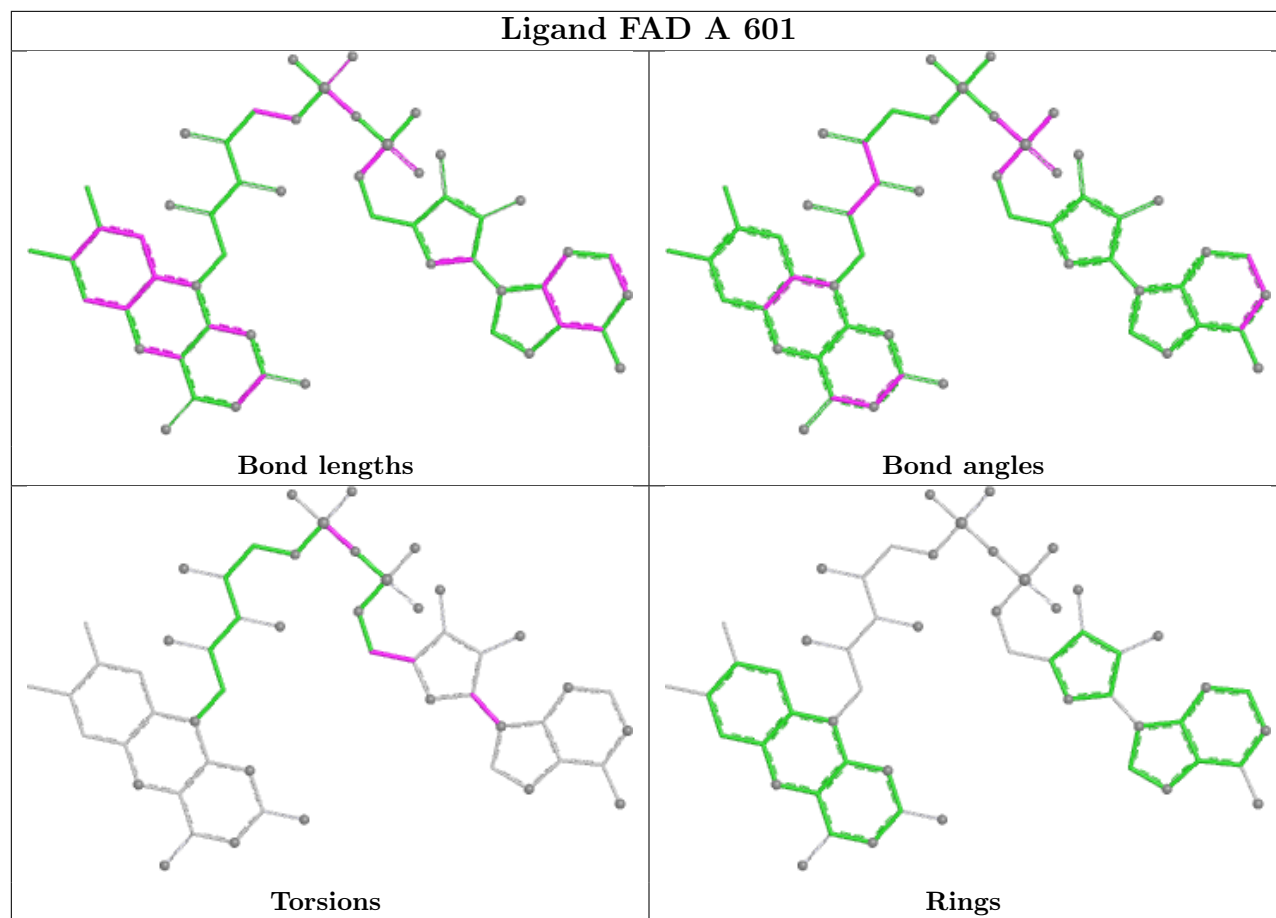
Ligand FAD C 603



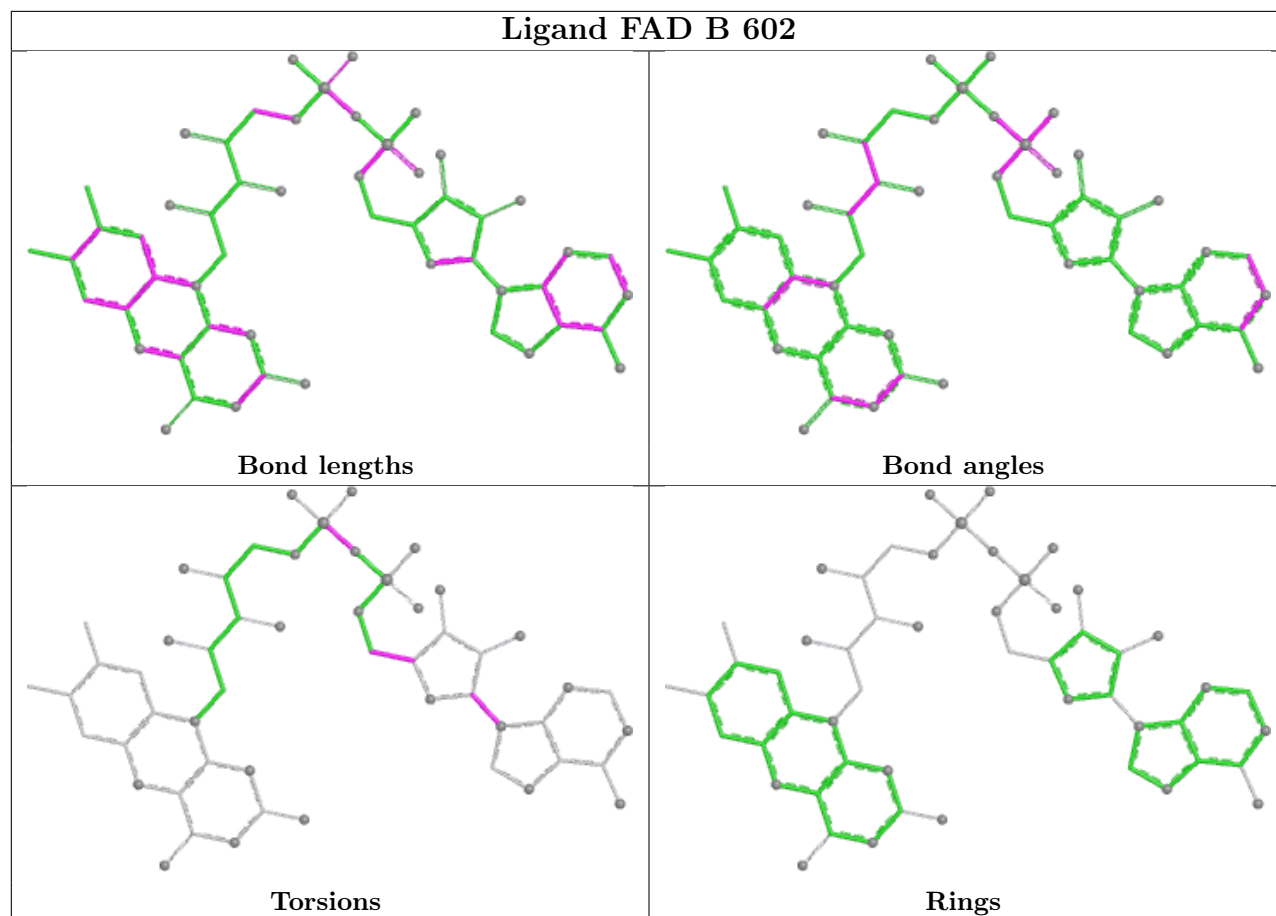
Ligand 936 B 704



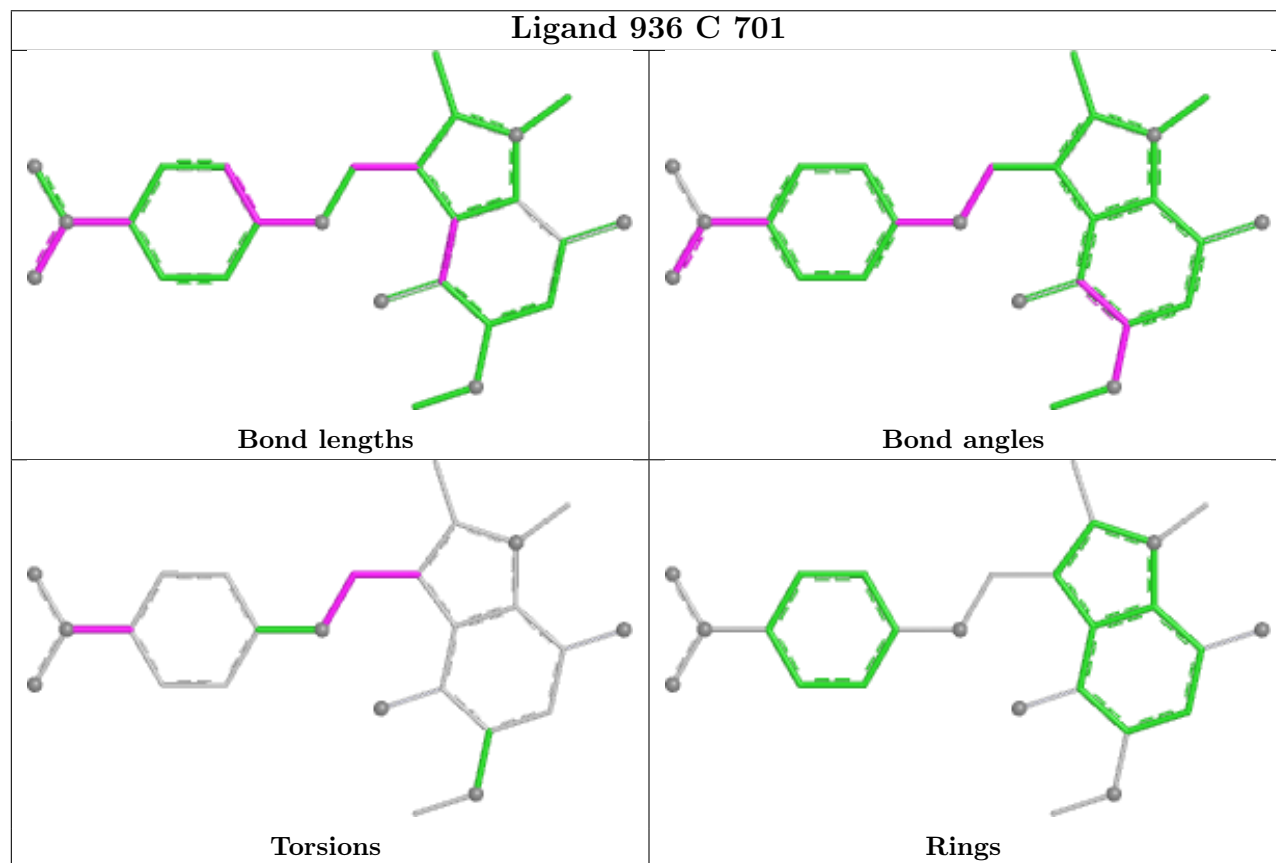
Ligand FAD A 601



Ligand FAD B 602



Ligand 936 C 701



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.