



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:21 AM UTC

PDB ID : 1ZPT / pdb_00001zpt
Title : Escherichia coli Methylenetetrahydrofolate Reductase (reduced) complexed with NADH, pH 7.25
Authors : Pejchal, R.; Sargeant, R.; Ludwig, M.L.
Deposited on : 2005-05-17
Resolution : 1.95 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

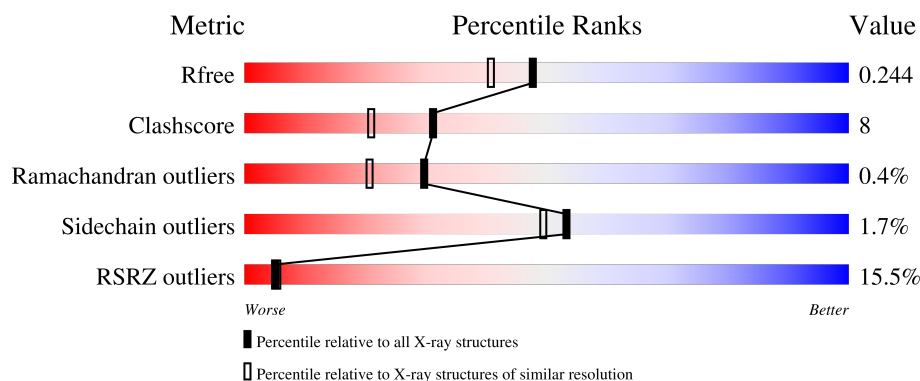
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	304	37% 66% 22% 11%
1	B	304	4% 82% 11% • 6%
1	C	304	2% 74% 12% • 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6953 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 5,10-methylenetetrahydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2068	1314	359	384	11			
1	B	285	Total	C	N	O	S	3	0	0
			2184	1380	379	414	11			
1	C	265	Total	C	N	O	S	0	0	0
			2064	1310	358	385	11			

There are 24 discrepancies between the modelled and reference sequences:

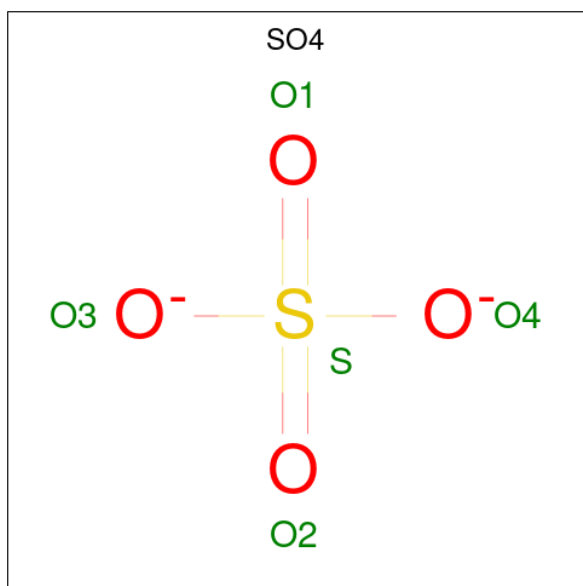
Chain	Residue	Modelled	Actual	Comment	Reference
A	297	LEU	-	cloning artifact	UNP P00394
A	298	GLU	-	cloning artifact	UNP P00394
A	299	HIS	-	expression tag	UNP P00394
A	300	HIS	-	expression tag	UNP P00394
A	301	HIS	-	expression tag	UNP P00394
A	302	HIS	-	expression tag	UNP P00394
A	303	HIS	-	expression tag	UNP P00394
A	304	HIS	-	expression tag	UNP P00394
B	297	LEU	-	cloning artifact	UNP P00394
B	298	GLU	-	cloning artifact	UNP P00394
B	299	HIS	-	expression tag	UNP P00394
B	300	HIS	-	expression tag	UNP P00394
B	301	HIS	-	expression tag	UNP P00394
B	302	HIS	-	expression tag	UNP P00394
B	303	HIS	-	expression tag	UNP P00394
B	304	HIS	-	expression tag	UNP P00394
C	297	LEU	-	cloning artifact	UNP P00394
C	298	GLU	-	cloning artifact	UNP P00394
C	299	HIS	-	expression tag	UNP P00394
C	300	HIS	-	expression tag	UNP P00394
C	301	HIS	-	expression tag	UNP P00394
C	302	HIS	-	expression tag	UNP P00394
C	303	HIS	-	expression tag	UNP P00394

Continued on next page...

Continued from previous page...

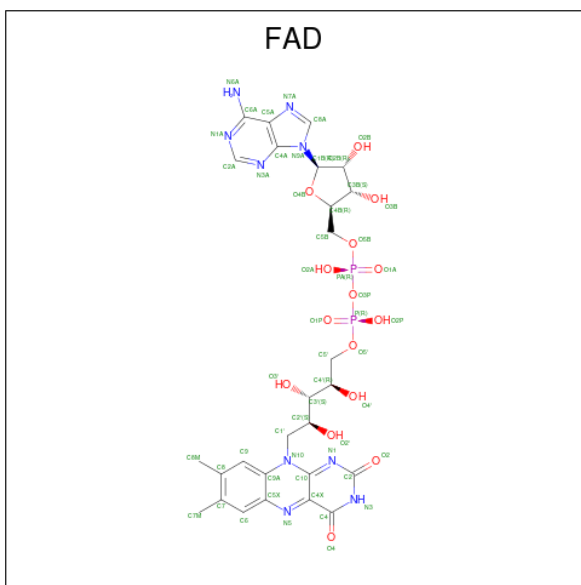
Chain	Residue	Modelled	Actual	Comment	Reference
C	304	HIS	-	expression tag	UNP P00394

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



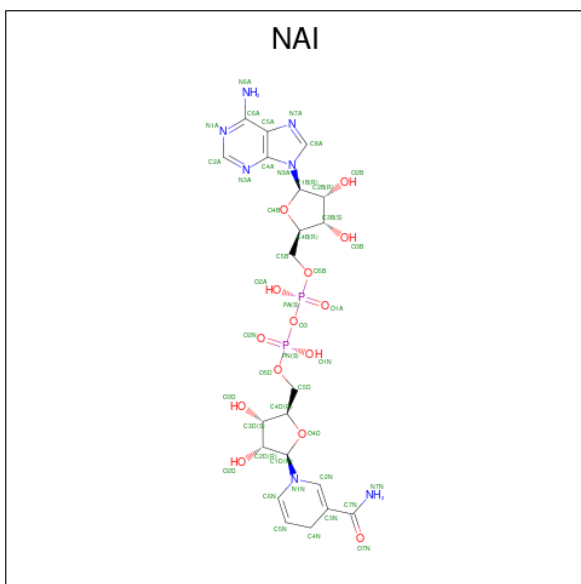
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	C	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $\text{C}_{21}\text{H}_{29}\text{N}_7\text{O}_{14}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	42	Total	O	0	0
			42	42		
5	B	128	Total	O	0	0
			128	128		
5	C	156	Total	O	0	0
			156	156		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.61Å 127.73Å 97.83Å 90.00° 121.73° 90.00°	Depositor
Resolution (Å)	19.90 – 1.95 19.90 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.90-1.95) 97.8 (19.90-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.246 0.218 , 0.244	Depositor DCC
R_{free} test set	3876 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6953	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	0/2109	0.81	3/2866 (0.1%)
1	B	0.39	0/2226	0.86	4/3023 (0.1%)
1	C	0.39	0/2106	0.88	8/2856 (0.3%)
All	All	0.37	0/6441	0.85	15/8745 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	GLN	N-CA-C	-9.13	98.48	110.53
1	C	146	ASP	N-CA-C	-8.13	95.97	109.46
1	C	183	GLN	N-CA-C	-7.99	99.98	110.53
1	A	183	GLN	N-CA-C	-7.36	100.13	110.50
1	B	146	ASP	N-CA-C	-7.35	97.26	109.46
1	A	215	SER	N-CA-C	-6.55	105.92	114.04
1	C	119	GLY	N-CA-C	-6.23	104.83	112.68
1	B	215	SER	N-CA-C	-6.15	106.32	113.88
1	B	214	VAL	N-CA-C	6.11	116.91	107.99
1	C	215	SER	N-CA-C	-5.57	107.12	114.31
1	C	204	ASP	N-CA-C	5.44	119.91	113.16
1	C	131	TYR	N-CA-C	-5.41	102.19	110.14
1	A	214	VAL	N-CA-C	5.24	116.24	108.23
1	C	213	PRO	N-CA-C	-5.03	103.20	110.80
1	C	274	PHE	N-CA-C	5.01	117.41	109.24

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	2068	0	1985	57	0
1	B	2184	0	2100	25	0
1	C	2064	0	2017	22	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
3	C	53	0	31	0	0
4	A	44	0	27	4	0
4	B	44	0	27	0	0
4	C	44	0	27	2	0
5	A	42	0	0	0	0
5	B	128	0	0	1	0
5	C	156	0	0	0	0
All	All	6953	0	6276	106	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 8.

All (106) 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:A:254:ALA:O	1:A:258:MET:HG2	1.61	0.99
1:B:238:MET:HE2	1:B:238:MET:HA	1.61	0.83
1:A:173:VAL:HA	1:A:177:ALA:HB3	1.64	0.79
1:A:89:LEU:HD23	1:A:135:LEU:HD11	1.67	0.77
1:A:258:MET:HE1	1:A:289:THR:OG1	1.87	0.75
1:A:74:ILE:HG13	1:A:87:PRO:HB3	1.68	0.74
1:A:258:MET:CE	1:A:289:THR:HG21	2.17	0.74
1:A:258:MET:HE1	1:A:289:THR:HG21	1.73	0.70
1:B:16:LEU:O	1:B:19:VAL:HG12	1.92	0.70
1:A:138:LEU:O	1:A:142:VAL:HG23	1.93	0.68
1:A:247:GLU:H	1:A:247:GLU:CD	2.01	0.68
1:C:112:ARG:HG2	1:C:112:ARG:HH21	1.60	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:MET:HE1	1:A:289:THR:CG2	2.25	0.67
1:B:34:THR:OG1	1:B:36:GLU:HG2	1.97	0.65
1:B:146:ASP:HA	1:B:178:ASN:HD21	1.60	0.65
1:C:238:MET:HG3	1:C:252:VAL:HG11	1.79	0.64
1:A:258:MET:HA	1:A:258:MET:HE3	1.79	0.64
1:B:137:THR:O	1:B:141:GLU:HG3	1.97	0.64
1:C:156:HIS:CD2	1:C:158:GLU:H	2.18	0.62
1:A:189:GLU:HB3	1:A:193:ARG:HH21	1.65	0.61
1:A:106:TYR:HB3	1:A:111:ILE:HB	1.83	0.61
1:B:67:ARG:HG2	1:B:67:ARG:HH21	1.67	0.59
1:A:100:ARG:HG2	1:A:138:LEU:HD21	1.83	0.59
1:A:32:PRO:HB3	1:A:37:MET:HG3	1.86	0.58
4:A:895:NAI:O5D	4:A:895:NAI:H6N	2.03	0.58
1:A:32:PRO:HD3	1:A:41:LEU:HD22	1.85	0.57
1:A:147:ILE:HD12	1:A:147:ILE:N	2.20	0.57
1:B:32:PRO:HD3	1:B:41:LEU:HD22	1.86	0.56
1:A:73:ILE:HD12	1:A:73:ILE:H	1.70	0.56
1:C:137:THR:O	1:C:141:GLU:HG3	2.05	0.56
1:B:36:GLU:H	1:B:36:GLU:CD	2.14	0.55
1:A:138:LEU:HA	1:A:141:GLU:HG2	1.88	0.55
1:A:54:LYS:HE3	1:A:179:ARG:HH12	1.73	0.54
1:A:73:ILE:HD12	1:A:73:ILE:N	2.22	0.54
1:A:138:LEU:C	1:A:138:LEU:HD23	2.33	0.54
1:C:222:LYS:O	1:C:226:MET:HG3	2.08	0.54
1:A:258:MET:HE1	1:A:289:THR:CB	2.38	0.53
1:C:120:ASP:OD2	4:C:897:NAI:H4D	2.09	0.53
1:A:143:ALA:HB3	1:A:145:PHE:CE1	2.43	0.53
1:C:238:MET:HG3	1:C:252:VAL:CG1	2.39	0.52
1:B:95:THR:OG1	1:B:98:GLU:HG3	2.08	0.52
1:B:163:GLN:HE21	1:B:163:GLN:H	1.57	0.52
1:C:90:THR:HA	1:C:117:LEU:O	2.10	0.52
1:A:247:GLU:CD	1:A:247:GLU:N	2.68	0.52
1:B:121:LEU:HD22	1:B:121:LEU:H	1.75	0.52
1:C:92:ILE:HG12	1:C:118:ARG:O	2.10	0.52
1:A:30:PHE:HB3	4:A:895:NAI:O2B	2.09	0.51
1:C:132:ALA:HB3	1:C:172:LYS:HD3	1.92	0.51
1:A:107:TRP:HB2	1:A:145:PHE:CZ	2.46	0.51
1:B:138:LEU:C	1:B:138:LEU:HD23	2.35	0.51
1:B:163:GLN:H	1:B:163:GLN:NE2	2.09	0.51
1:A:98:GLU:O	1:A:102:ILE:HG12	2.10	0.51
1:A:90:THR:HA	1:A:117:LEU:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ALA:HB3	1:A:172:LYS:HD3	1.94	0.50
1:C:140:LYS:HD3	1:C:147:ILE:HD12	1.94	0.50
1:A:41:LEU:HD13	1:A:278:ASN:CG	2.37	0.50
1:B:96:PRO:O	1:B:100:ARG:HG3	2.12	0.49
1:A:96:PRO:O	1:A:100:ARG:HG3	2.12	0.49
1:A:199:VAL:HG23	1:A:200:SER:N	2.26	0.49
1:A:108:ASN:C	1:A:109:ASN:HD22	2.21	0.49
1:B:121:LEU:HD22	1:B:121:LEU:N	2.27	0.49
1:B:33:ARG:HD3	5:B:567:HOH:O	2.13	0.49
1:C:156:HIS:HD2	1:C:158:GLU:H	1.61	0.48
1:A:258:MET:HE3	1:A:258:MET:CA	2.37	0.48
1:B:238:MET:HA	1:B:238:MET:CE	2.39	0.48
1:A:135:LEU:O	1:A:135:LEU:HD13	2.14	0.48
1:A:251:LEU:HD23	1:C:251:LEU:HD23	1.96	0.47
1:C:112:ARG:HG2	1:C:112:ARG:NH2	2.27	0.47
1:C:215:SER:HB3	1:C:282:MET:SD	2.54	0.47
1:A:188:VAL:HG22	1:A:260:MET:HG3	1.97	0.46
1:A:287:CYS:HB3	1:A:292:VAL:HB	1.97	0.46
1:B:33:ARG:HH12	1:B:66:GLU:CD	2.22	0.46
1:B:16:LEU:HD11	1:B:290:LEU:HD23	1.98	0.46
1:A:138:LEU:O	1:A:141:GLU:HG2	2.16	0.46
1:C:34:THR:OG1	1:C:36:GLU:HG2	2.16	0.46
1:A:40:THR:HG21	1:A:279:ARG:HH11	1.80	0.46
1:B:94:ALA:HB3	1:B:99:LEU:HD21	1.98	0.45
1:A:116:ALA:HB1	1:A:135:LEU:HD12	2.00	0.44
4:A:895:NAI:H2B	4:A:895:NAI:H42N	2.00	0.43
1:A:73:ILE:O	1:A:77:ILE:HG13	2.19	0.43
1:A:182:THR:CG2	1:A:207:ILE:HG22	2.48	0.43
1:B:32:PRO:HD3	1:B:41:LEU:CD2	2.49	0.43
1:C:138:LEU:C	1:C:138:LEU:HD23	2.44	0.43
1:B:186:PHE:CE2	1:B:235:MET:HE1	2.53	0.42
1:C:218:LYS:HA	1:C:218:LYS:HE3	2.00	0.42
1:A:107:TRP:HB2	1:A:145:PHE:CE2	2.54	0.42
1:B:41:LEU:O	1:B:45:ILE:HG12	2.19	0.42
1:A:267:GLU:HA	1:A:267:GLU:OE1	2.20	0.42
1:C:96:PRO:O	1:C:100:ARG:HG3	2.18	0.42
1:A:169:LEU:O	1:A:173:VAL:HG23	2.20	0.42
1:A:184:PHE:CE1	1:A:229:VAL:HG11	2.55	0.42
1:B:67:ARG:NH2	1:B:102:ILE:HD11	2.34	0.41
1:A:20:GLN:HA	1:A:291:GLY:HA3	2.01	0.41
1:A:184:PHE:CD1	1:A:184:PHE:C	2.98	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:HG2	1:A:193:ARG:HH11	1.85	0.41
4:A:895:NAI:O5B	4:A:895:NAI:H8A	2.20	0.41
1:C:30:PHE:HB3	4:C:897:NAI:O2B	2.20	0.41
1:B:260:MET:HE2	1:B:260:MET:HB3	1.98	0.41
1:A:60:TYR:CD1	1:A:60:TYR:C	2.98	0.41
1:C:173:VAL:HA	1:C:177:ALA:HB3	2.02	0.41
1:A:73:ILE:H	1:A:73:ILE:CD1	2.32	0.41
1:A:74:ILE:HG23	1:A:85:ALA:HB3	2.03	0.41
1:A:136:VAL:HG13	1:A:147:ILE:HG21	2.02	0.41
1:A:116:ALA:CB	1:A:135:LEU:HD12	2.51	0.41
1:A:140:LYS:C	1:A:142:VAL:H	2.29	0.40
1:C:214:VAL:O	1:C:253:GLY:HA3	2.21	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	265/304 (87%)	259 (98%)	5 (2%)	1 (0%)	30	21
1	B	281/304 (92%)	278 (99%)	2 (1%)	1 (0%)	30	21
1	C	261/304 (86%)	253 (97%)	7 (3%)	1 (0%)	30	21
All	All	807/912 (88%)	790 (98%)	14 (2%)	3 (0%)	30	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	VAL
1	B	155	VAL
1	C	155	VAL

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	210/258 (81%)	206 (98%)	4 (2%)	50	45
1	B	225/258 (87%)	219 (97%)	6 (3%)	39	32
1	C	217/258 (84%)	216 (100%)	1 (0%)	81	82
All	All	652/774 (84%)	641 (98%)	11 (2%)	53	49

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ARG
1	A	118	ARG
1	A	130	MET
1	A	193	ARG
1	B	36	GLU
1	B	163	GLN
1	B	167	LEU
1	B	206	GLU
1	B	228	ASN
1	B	238	MET
1	C	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	39	GLN
1	A	43	ASN
1	A	109	ASN
1	A	178	ASN
1	A	228	ASN
1	B	14	GLN
1	B	20	GLN
1	B	163	GLN
1	B	178	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	228	ASN
1	C	156	HIS

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 ⓘ

10 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	SO4	A	899	-	4,4,4	0.35	0	6,6,6	0.06	0
4	NAI	B	896	-	47,48,48	1.59	11 (23%)	64,73,73	1.50	9 (14%)
3	FAD	C	397	-	58,58,58	1.55	8 (13%)	85,89,89	1.26	11 (12%)
3	FAD	B	396	-	58,58,58	1.57	10 (17%)	85,89,89	1.29	15 (17%)
4	NAI	A	895	-	47,48,48	1.56	11 (23%)	64,73,73	1.54	9 (14%)
2	SO4	A	900	-	4,4,4	0.36	0	6,6,6	0.07	0
2	SO4	B	901	-	4,4,4	0.37	0	6,6,6	0.07	0
4	NAI	C	897	-	47,48,48	1.55	10 (21%)	64,73,73	1.56	10 (15%)
2	SO4	C	902	-	4,4,4	0.35	0	6,6,6	0.08	0
3	FAD	A	395	-	58,58,58	1.71	11 (18%)	85,89,89	1.46	14 (16%)

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
4	NAI	B	896	-	-	4/29/72/72	0/5/5/5
3	FAD	C	397	-	-	2/34/50/50	0/6/6/6
3	FAD	B	396	-	-	3/34/50/50	0/6/6/6
4	NAI	A	895	-	-	5/29/72/72	0/5/5/5
4	NAI	C	897	-	-	6/29/72/72	0/5/5/5
3	FAD	A	395	-	-	6/34/50/50	0/6/6/6

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	395	FAD	C10-N10	5.61	1.49	1.37
3	A	395	FAD	C9A-N10	4.78	1.49	1.41
4	B	896	NAI	C4N-C3N	-4.70	1.41	1.50
4	A	895	NAI	C4N-C3N	-4.67	1.41	1.50
4	C	897	NAI	C4N-C3N	-4.66	1.41	1.50
3	C	397	FAD	C4X-N5	4.64	1.40	1.30
3	B	396	FAD	C4X-N5	4.58	1.40	1.30
3	C	397	FAD	C10-N10	4.54	1.47	1.37
3	A	395	FAD	C4X-N5	4.49	1.40	1.30
3	B	396	FAD	C10-N10	4.36	1.46	1.37
3	B	396	FAD	C9A-N10	4.26	1.48	1.41
3	A	395	FAD	C9-C9A	3.94	1.46	1.39
3	C	397	FAD	C9A-N10	3.84	1.47	1.41
3	C	397	FAD	C9-C9A	3.61	1.45	1.39
3	B	396	FAD	C6-C5X	3.38	1.45	1.40
4	A	895	NAI	C5A-N7A	-3.29	1.33	1.39
4	C	897	NAI	C5A-N7A	-3.26	1.33	1.39
3	B	396	FAD	C9-C9A	3.24	1.44	1.39
4	B	896	NAI	C5A-N7A	-3.22	1.33	1.39
3	B	396	FAD	C8-C7	3.17	1.48	1.40
4	A	895	NAI	C4N-C5N	-3.15	1.40	1.49
4	C	897	NAI	C4N-C5N	-3.13	1.40	1.49
4	B	896	NAI	C4N-C5N	-3.09	1.41	1.49
3	A	395	FAD	C8-C7	3.03	1.48	1.40
4	B	896	NAI	PN-O3	3.01	1.62	1.59
3	A	395	FAD	C5'-C4'	3.01	1.55	1.51
3	A	395	FAD	C6-C5X	2.97	1.44	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	896	NAI	O4B-C1B	2.96	1.48	1.42
4	C	897	NAI	O4B-C1B	2.94	1.48	1.42
4	B	896	NAI	O4D-C1D	2.93	1.48	1.42
4	A	895	NAI	O4B-C1B	2.93	1.48	1.42
3	C	397	FAD	C6-C5X	2.89	1.44	1.40
3	C	397	FAD	C8-C7	2.86	1.47	1.40
3	B	396	FAD	P-O3P	2.82	1.62	1.59
3	A	395	FAD	P-O3P	2.77	1.62	1.59
3	A	395	FAD	C1'-C2'	2.74	1.56	1.52
4	A	895	NAI	C7N-C3N	2.54	1.54	1.48
4	A	895	NAI	O4D-C1D	2.52	1.47	1.42
4	C	897	NAI	PN-O3	2.52	1.62	1.59
4	B	896	NAI	C7N-C3N	2.51	1.54	1.48
3	B	396	FAD	C9A-C5X	2.45	1.45	1.41
4	B	896	NAI	C6N-C5N	2.45	1.40	1.33
4	C	897	NAI	C6N-C5N	2.41	1.40	1.33
4	A	895	NAI	C6N-C5N	2.40	1.40	1.33
4	C	897	NAI	C7N-C3N	2.39	1.53	1.48
3	C	397	FAD	C9A-C5X	2.38	1.45	1.41
3	A	395	FAD	C10-N1	2.36	1.38	1.33
4	A	895	NAI	PN-O3	2.34	1.62	1.59
3	B	396	FAD	C7M-C7	2.34	1.55	1.51
4	B	896	NAI	PA-O3	2.26	1.61	1.59
4	C	897	NAI	O4D-C1D	2.24	1.47	1.42
4	C	897	NAI	C6N-N1N	2.23	1.42	1.37
4	C	897	NAI	PA-O3	2.22	1.61	1.59
4	A	895	NAI	C6N-N1N	2.20	1.42	1.37
4	B	896	NAI	C6N-N1N	2.20	1.42	1.37
3	C	397	FAD	C2'-C3'	2.20	1.57	1.53
4	A	895	NAI	PA-O3	2.15	1.61	1.59
4	A	895	NAI	C2N-C3N	2.08	1.40	1.35
4	B	896	NAI	C4A-N9A	-2.05	1.33	1.37
3	A	395	FAD	C9A-C5X	2.03	1.44	1.41
3	B	396	FAD	C10-N1	2.01	1.37	1.33

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	896	NAI	N3A-C2A-N1A	-5.35	120.48	128.58
4	A	895	NAI	N3A-C2A-N1A	-5.31	120.55	128.58
4	C	897	NAI	N3A-C2A-N1A	-5.28	120.58	128.58
4	A	895	NAI	C5A-C4A-N3A	-5.04	119.78	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	897	NAI	C5A-C4A-N3A	-5.02	119.80	126.72
3	A	395	FAD	C5'-C4'-C3'	4.93	121.51	112.22
4	B	896	NAI	C5A-C4A-N3A	-4.89	119.99	126.72
3	C	397	FAD	C5X-C9A-N10	-3.96	114.39	117.97
3	A	395	FAD	C5X-C9A-N10	-3.93	114.42	117.97
3	A	395	FAD	C9-C9A-N10	3.86	127.05	121.85
3	A	395	FAD	C9A-C5X-N5	3.75	126.43	122.45
4	A	895	NAI	C2A-N3A-C4A	3.69	120.84	111.83
4	C	897	NAI	C2A-N3A-C4A	3.69	120.83	111.83
4	B	896	NAI	C2A-N3A-C4A	3.66	120.76	111.83
3	C	397	FAD	C9-C9A-N10	3.56	126.64	121.85
3	A	395	FAD	C4'-C3'-C2'	3.44	119.29	113.57
4	B	896	NAI	N9A-C8A-N7A	-3.43	109.07	113.94
4	C	897	NAI	N3A-C4A-N9A	3.41	132.97	127.17
4	C	897	NAI	N9A-C8A-N7A	-3.39	109.13	113.94
4	A	895	NAI	N3A-C4A-N9A	3.37	132.91	127.17
4	A	895	NAI	N9A-C8A-N7A	-3.36	109.17	113.94
4	B	896	NAI	N3A-C4A-N9A	3.31	132.79	127.17
3	B	396	FAD	C5X-C9A-N10	-3.30	114.99	117.97
3	B	396	FAD	O2-C2-N3	3.27	124.85	118.58
4	C	897	NAI	O4D-C1D-N1N	3.24	114.26	108.08
4	A	895	NAI	O4D-C1D-N1N	2.88	113.57	108.08
4	C	897	NAI	C5A-N7A-C8A	2.86	107.94	103.45
4	A	895	NAI	C5A-N7A-C8A	2.81	107.87	103.45
3	C	397	FAD	C9A-C5X-N5	2.79	125.42	122.45
3	B	396	FAD	C5'-C4'-C3'	2.79	117.48	112.22
4	B	896	NAI	C5A-N7A-C8A	2.76	107.79	103.45
3	C	397	FAD	O2-C2-N3	2.74	123.85	118.58
3	B	396	FAD	C9-C9A-N10	2.70	125.48	121.85
3	B	396	FAD	O5'-C5'-C4'	2.64	116.40	109.36
3	C	397	FAD	O5'-C5'-C4'	2.61	116.33	109.36
3	B	396	FAD	C8M-C8-C9	-2.60	114.99	119.57
3	A	395	FAD	O2'-C2'-C3'	2.58	115.28	109.25
3	B	396	FAD	C9A-C5X-N5	2.53	125.14	122.45
4	A	895	NAI	C3N-C2N-N1N	-2.45	119.60	123.20
3	B	396	FAD	O3'-C3'-C4'	2.43	114.46	108.93
3	B	396	FAD	C8M-C8-C7	2.43	125.71	120.76
4	A	895	NAI	C4A-C5A-N7A	-2.41	107.83	110.58
4	C	897	NAI	C4A-C5A-N7A	-2.40	107.83	110.58
3	B	396	FAD	O5B-C5B-C4B	2.40	117.17	108.99
3	A	395	FAD	O5'-C5'-C4'	2.38	115.72	109.36
4	C	897	NAI	C3N-C2N-N1N	-2.38	119.71	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	397	FAD	C8M-C8-C7	2.33	125.51	120.76
3	A	395	FAD	C8M-C8-C7	2.33	125.51	120.76
3	B	396	FAD	N3-C2-N1	-2.32	114.57	119.50
4	B	896	NAI	C4A-C5A-N7A	-2.30	107.95	110.58
4	B	896	NAI	C3N-C2N-N1N	-2.28	119.86	123.20
3	C	397	FAD	N3-C2-N1	-2.25	114.72	119.50
3	A	395	FAD	C6-C5X-N5	-2.23	114.74	118.44
3	A	395	FAD	C7M-C7-C6	-2.22	115.66	119.57
3	B	396	FAD	C10-N1-C2	2.20	121.61	116.85
3	A	395	FAD	C8M-C8-C9	-2.20	115.70	119.57
3	A	395	FAD	C7M-C7-C8	2.19	125.24	120.76
3	C	397	FAD	O2B-C2B-C1B	2.19	117.64	110.10
3	C	397	FAD	C10-N1-C2	2.13	121.45	116.85
4	B	896	NAI	C4A-N9A-C8A	2.12	107.97	105.74
3	B	396	FAD	O2'-C2'-C3'	2.11	114.19	109.25
3	B	396	FAD	C1B-N9A-C8A	2.11	131.77	127.09
3	C	397	FAD	C8M-C8-C9	-2.09	115.90	119.57
3	A	395	FAD	O2B-C2B-C1B	2.06	117.20	110.10
3	A	395	FAD	C4-C4X-N5	-2.06	115.36	118.21
3	C	397	FAD	O3P-PA-O1A	-2.05	104.54	110.70
3	B	396	FAD	O2B-C2B-C1B	2.02	117.06	110.10
4	C	897	NAI	C4A-N9A-C8A	2.02	107.86	105.74

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	895	NAI	C5B-O5B-PA-O1A
4	A	895	NAI	C5B-O5B-PA-O2A
4	A	895	NAI	C5B-O5B-PA-O3
4	B	896	NAI	C5B-O5B-PA-O1A
4	B	896	NAI	C5B-O5B-PA-O2A
4	B	896	NAI	C5B-O5B-PA-O3
4	B	896	NAI	O4D-C1D-N1N-C2N
4	C	897	NAI	C5B-O5B-PA-O1A
4	C	897	NAI	C5B-O5B-PA-O2A
4	C	897	NAI	C5B-O5B-PA-O3
3	A	395	FAD	O4'-C4'-C5'-O5'
3	A	395	FAD	O2'-C2'-C3'-C4'
4	C	897	NAI	O4D-C1D-N1N-C2N
3	B	396	FAD	O2'-C2'-C3'-C4'
3	C	397	FAD	O2'-C2'-C3'-C4'

Continued on next page...

Continued from previous page...

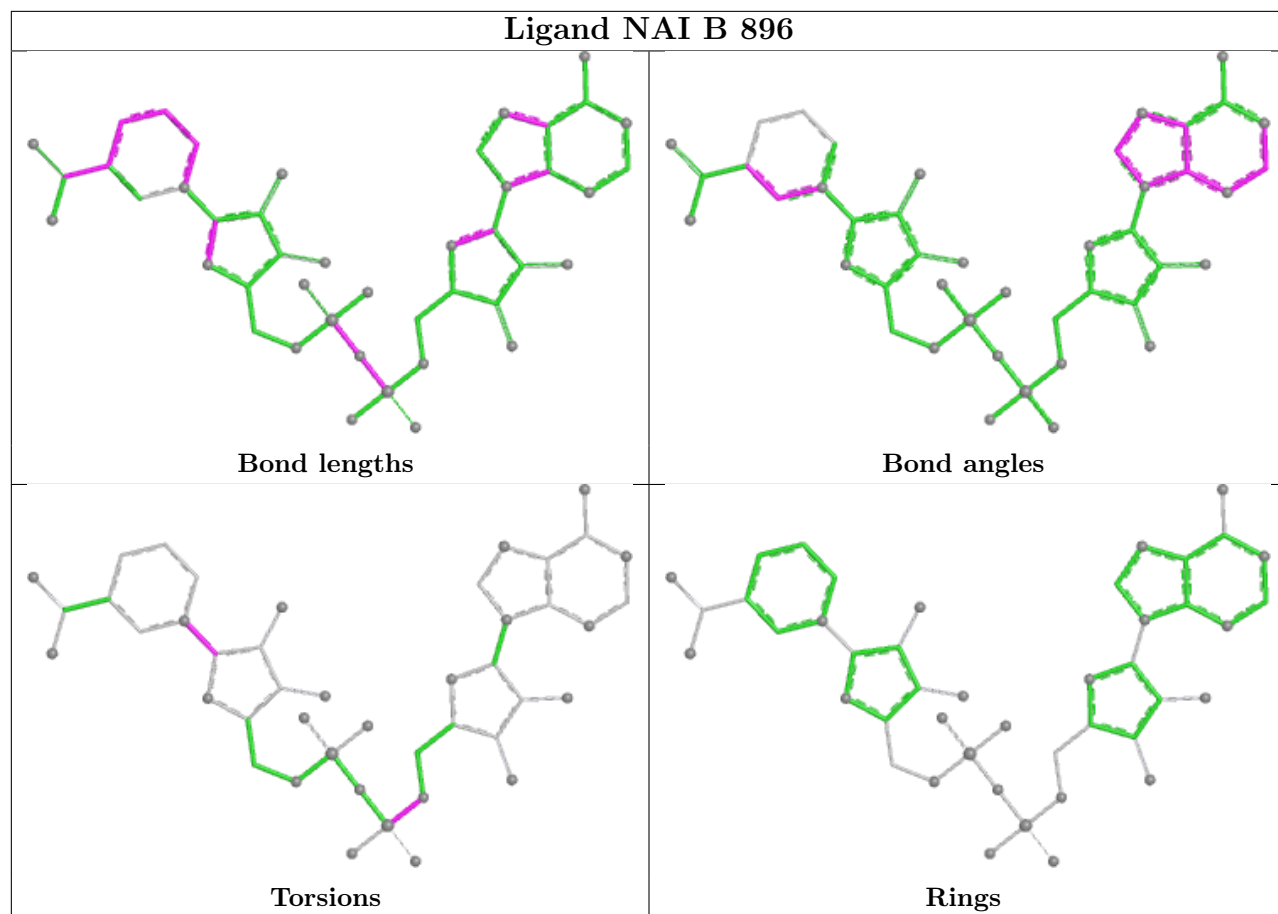
Mol	Chain	Res	Type	Atoms
4	A	895	NAI	O4D-C1D-N1N-C2N
3	A	395	FAD	C5B-O5B-PA-O1A
4	C	897	NAI	C5D-O5D-PN-O1N
3	A	395	FAD	PA-O3P-P-O2P
3	B	396	FAD	P-O3P-PA-O1A
3	A	395	FAD	C2'-C3'-C4'-C5'
4	A	895	NAI	C2N-C3N-C7N-N7N
4	C	897	NAI	C2N-C3N-C7N-N7N
3	B	396	FAD	P-O3P-PA-O2A
3	C	397	FAD	C2'-C3'-C4'-O4'
3	A	395	FAD	O3'-C3'-C4'-C5'

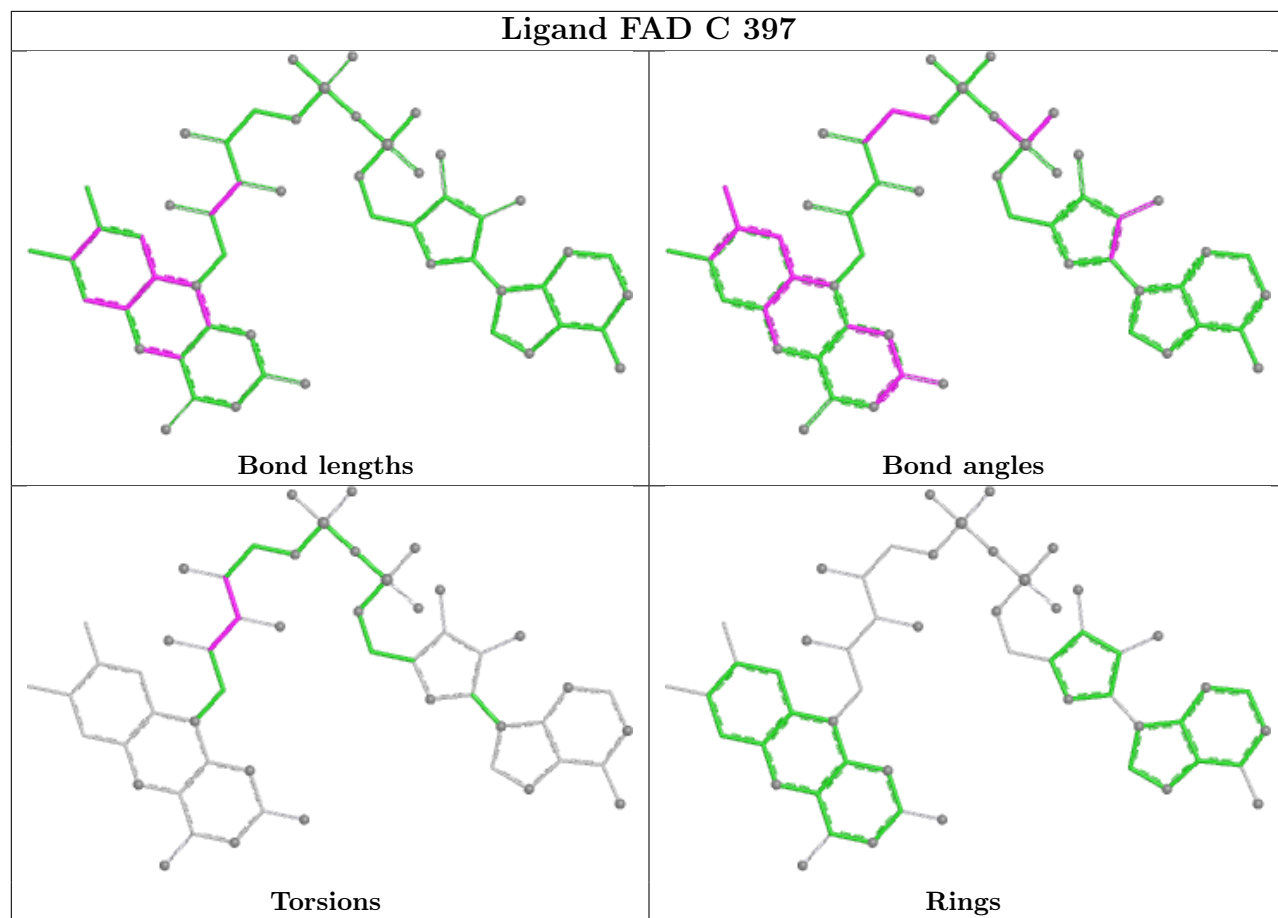
There are no ring outliers.

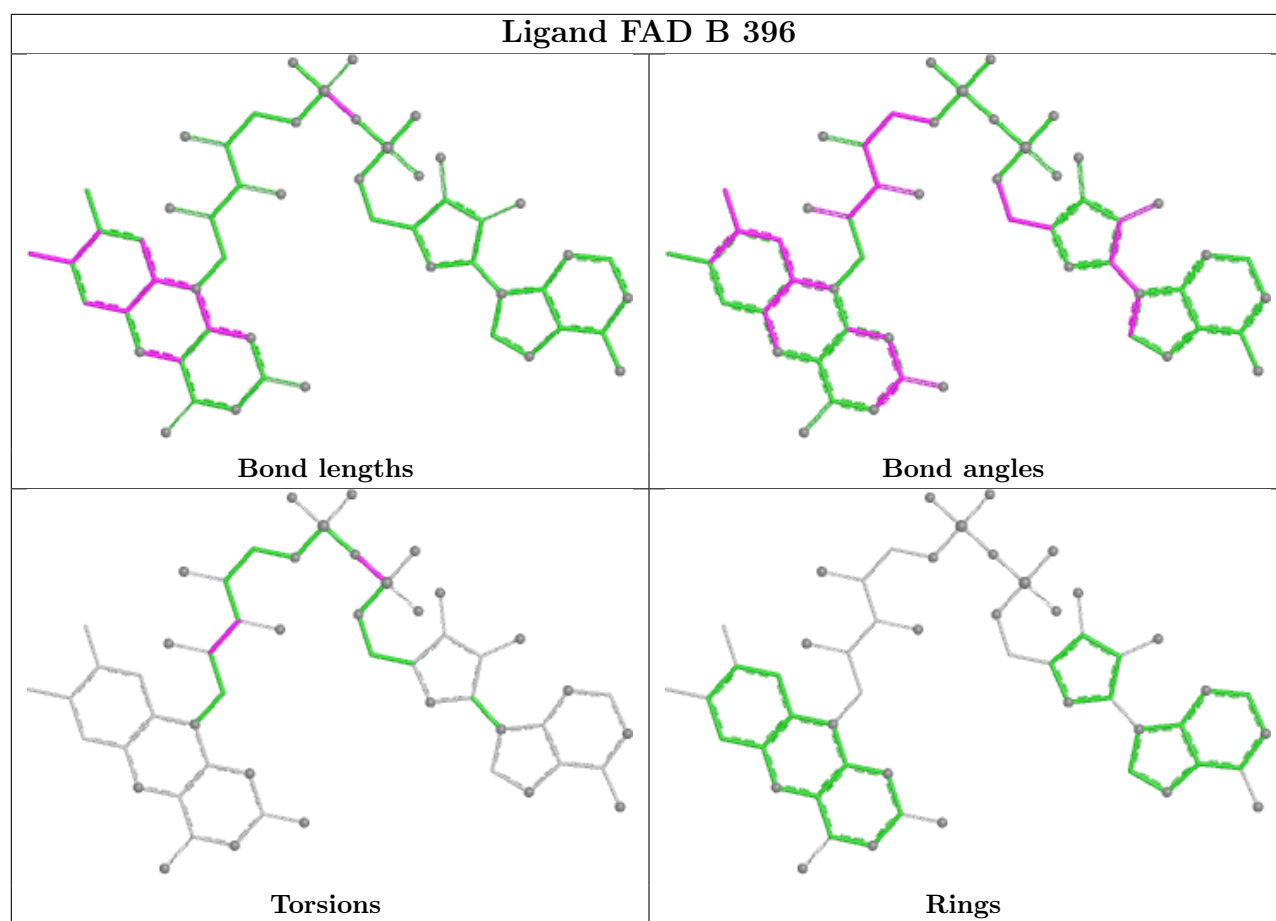
2 monomers are involved in 6 short contacts:

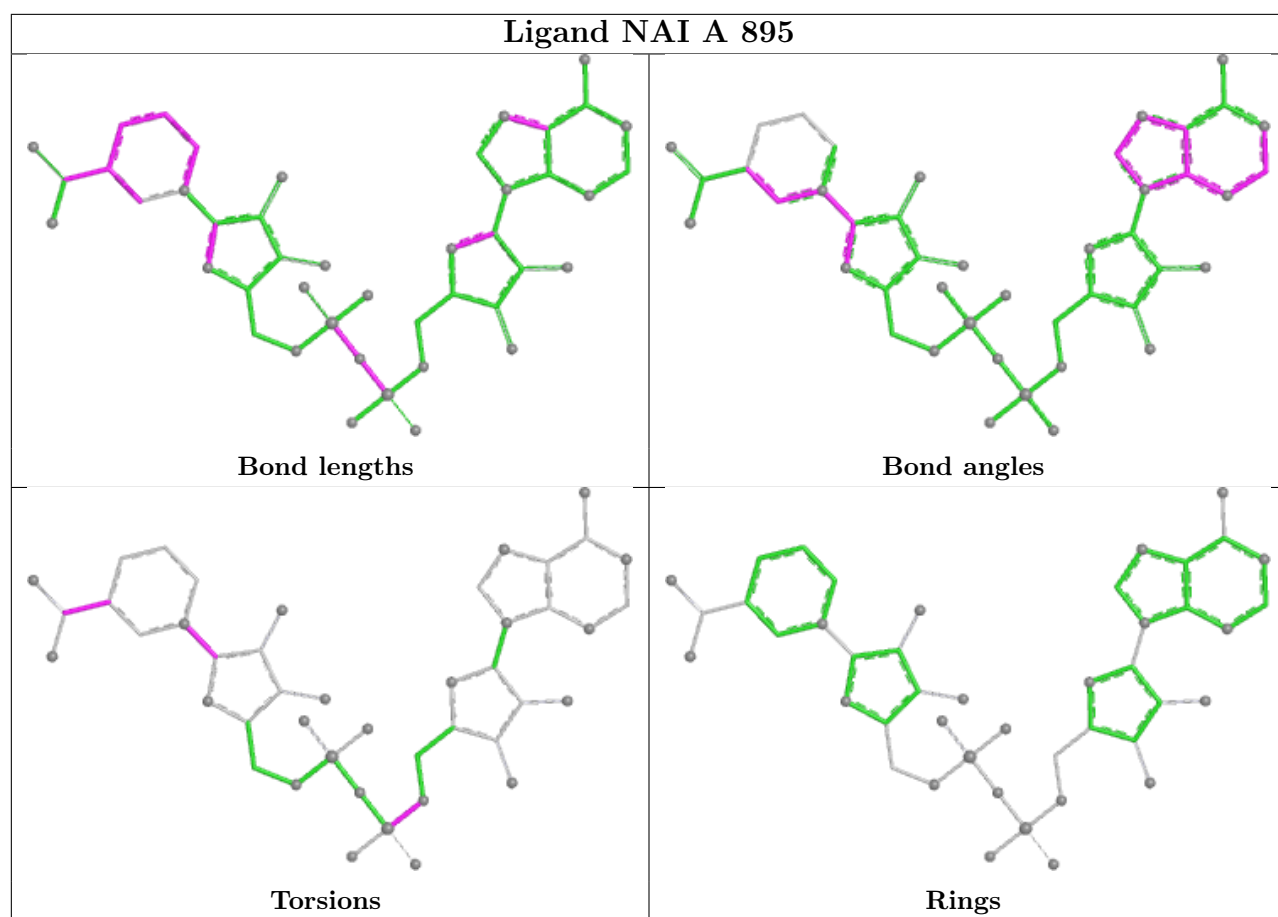
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	895	NAI	4	0
4	C	897	NAI	2	0

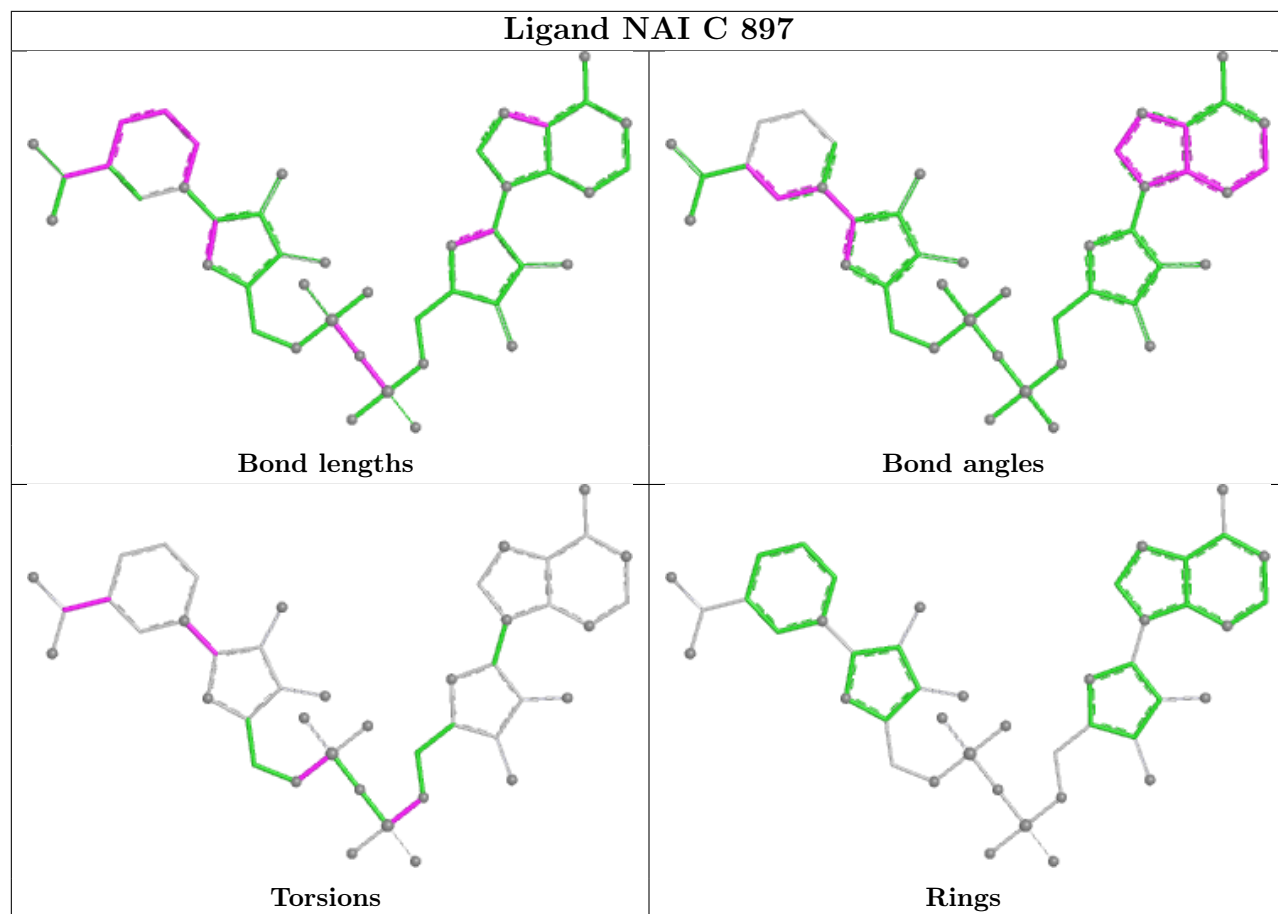
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

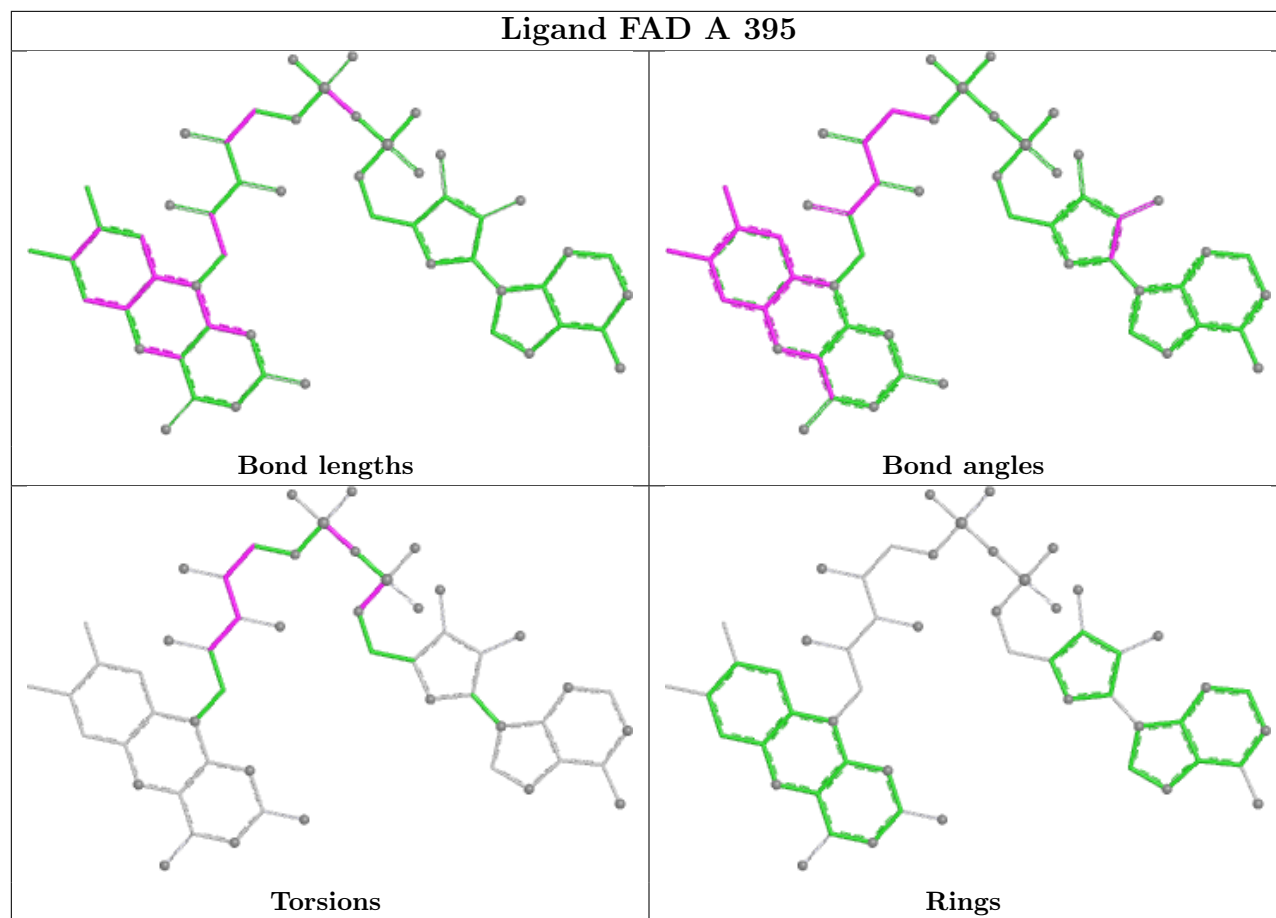












5.7 Other polymers [i](#)

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	271/304 (89%)	1.89	111 (40%) 0 0	22, 45, 72, 80	0
1	B	285/304 (93%)	0.36	11 (3%) 43 50	16, 27, 41, 49	1 (0%)
1	C	265/304 (87%)	0.05	5 (1%) 66 74	16, 24, 36, 47	0
All	All	821/912 (90%)	0.76	127 (15%) 5 5	16, 30, 62, 80	1 (0%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	ILE	6.4
1	A	92	ILE	6.2
1	A	114	ILE	5.9
1	B	3	PHE	5.7
1	B	62	ALA	5.4
1	A	258	MET	5.2
1	A	106	TYR	5.0
1	A	143	ALA	4.9
1	A	201	ALA	4.9
1	A	145	PHE	4.8
1	A	89	LEU	4.6
1	A	99	LEU	4.6
1	A	101	THR	4.5
1	A	70	THR	4.4
1	A	136	VAL	4.4
1	B	121	LEU	4.4
1	A	110	GLY	4.3
1	A	135	LEU	4.3
1	A	146	ASP	4.2
1	A	131	TYR	4.1
1	A	107	TRP	4.1
1	A	60	TYR	4.1
1	A	132	ALA	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	140	LYS	4.0
1	A	95	THR	3.9
1	A	142	VAL	3.9
1	A	147	ILE	3.9
1	A	115	VAL	3.9
1	A	148	SER	3.8
1	A	139	LEU	3.8
1	A	175	ALA	3.8
1	A	138	LEU	3.7
1	A	166	LEU	3.7
1	A	77	ILE	3.7
1	A	73	ILE	3.7
1	A	74	ILE	3.6
1	A	199	VAL	3.6
1	A	19	VAL	3.6
1	A	133	SER	3.6
1	A	108	ASN	3.5
1	A	141	GLU	3.5
1	A	202	GLY	3.5
1	B	21	GLY	3.5
1	A	117	LEU	3.5
1	A	91	CYS	3.4
1	A	94	ALA	3.4
1	A	111	ILE	3.4
1	A	180	ALA	3.4
1	A	159	ALA	3.3
1	A	97	ASP	3.3
1	A	167	LEU	3.3
1	A	105	ASP	3.3
1	A	7	SER	3.3
1	A	103	ALA	3.2
1	A	116	ALA	3.2
1	A	130	MET	3.2
1	A	93	ASP	3.2
1	A	83	LEU	3.1
1	A	78	LYS	3.1
1	A	137	THR	3.1
1	A	96	PRO	3.1
1	A	164	ALA	3.0
1	A	165	ASP	3.0
1	A	162	ALA	2.9
1	A	150	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	228	ASN	2.8
1	A	179	ARG	2.8
1	A	104	ARG	2.8
1	A	161	SER	2.8
1	B	228	ASN	2.8
1	A	23	ILE	2.8
1	A	169	LEU	2.8
1	A	200	SER	2.8
1	C	65	GLY	2.8
1	A	144	ASP	2.7
1	A	149	VAL	2.7
1	A	193	ARG	2.7
1	A	81	THR	2.7
1	B	93	ASP	2.7
1	A	163	GLN	2.6
1	A	226	MET	2.6
1	A	177	ALA	2.6
1	A	152	TYR	2.6
1	A	90	THR	2.6
1	A	82	GLY	2.5
1	A	188	VAL	2.5
1	A	42	TRP	2.5
1	A	80	ARG	2.5
1	A	113	HIS	2.5
1	C	266	ARG	2.5
1	A	204	ASP	2.5
1	A	155	VAL	2.5
1	A	178	ASN	2.4
1	A	55	PHE	2.4
1	A	194	PHE	2.4
1	A	157	PRO	2.4
1	A	5	HIS	2.4
1	A	174	ASP	2.4
1	A	119	GLY	2.4
1	B	226	MET	2.4
1	A	225	ASP	2.4
1	A	71	HIS	2.4
1	A	21	GLY	2.4
1	A	173	VAL	2.4
1	A	72	SER	2.4
1	A	134	ASP	2.3
1	A	168	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	112	ARG	2.3
1	C	22	GLN	2.3
1	A	171	ARG	2.3
1	B	19	VAL	2.3
1	A	198	CYS	2.3
1	C	227	THR	2.3
1	A	109	ASN	2.2
1	A	41	LEU	2.2
1	A	98	GLU	2.2
1	A	224	ALA	2.2
1	A	269	VAL	2.2
1	A	234	TRP	2.2
1	B	39	GLN	2.2
1	A	118	ARG	2.2
1	A	172	LYS	2.2
1	A	20	GLN	2.1
1	B	4	PHE	2.1
1	B	5	HIS	2.1
1	A	58	VAL	2.0
1	A	227	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAI	A	895	44/44	0.70	0.21	72,74,79,79	44
4	NAI	B	896	44/44	0.75	0.17	37,46,55,56	44
4	NAI	C	897	44/44	0.80	0.15	40,45,55,56	44

Continued on next page...

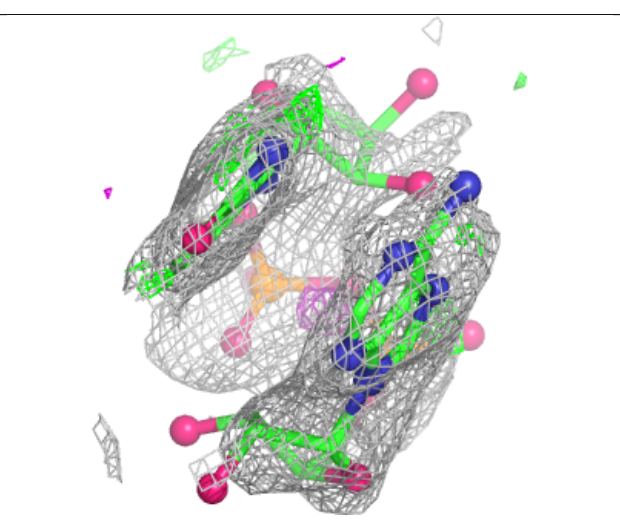
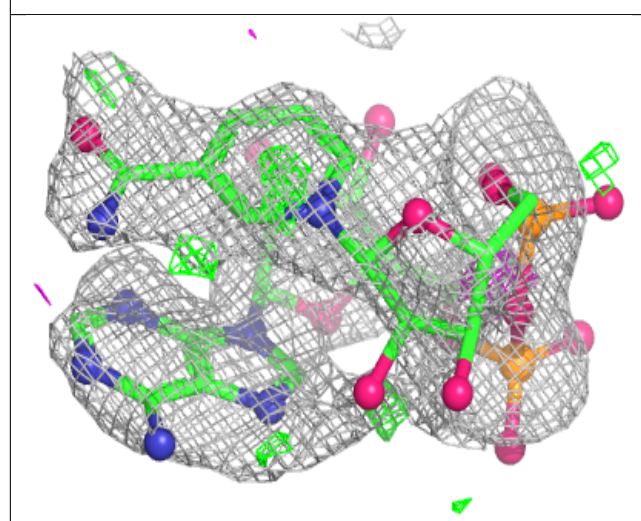
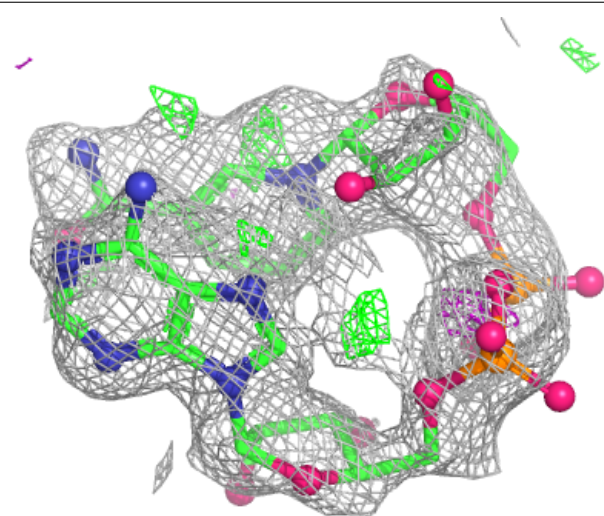
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FAD	A	395	53/53	0.84	0.14	39,46,59,60	0
2	SO4	B	901	5/5	0.88	0.17	45,46,46,46	5
2	SO4	A	899	5/5	0.89	0.11	56,56,56,56	5
2	SO4	C	902	5/5	0.90	0.13	50,50,51,51	5
2	SO4	A	900	5/5	0.91	0.12	62,62,62,62	5
3	FAD	B	396	53/53	0.96	0.07	21,25,33,33	0
3	FAD	C	397	53/53	0.98	0.05	18,21,29,29	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.

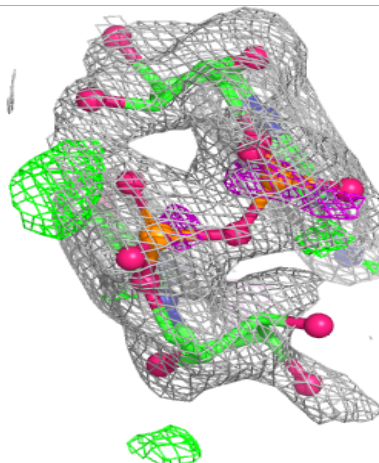
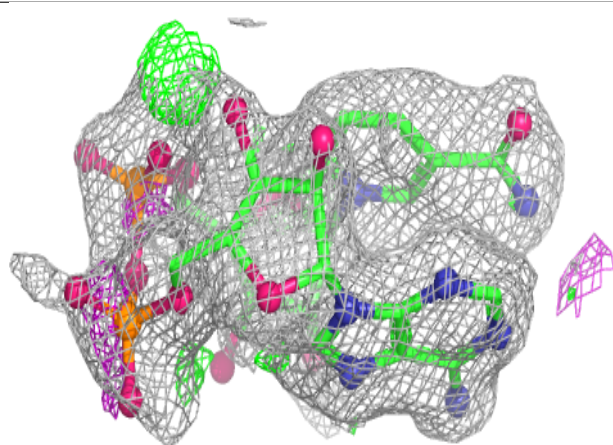
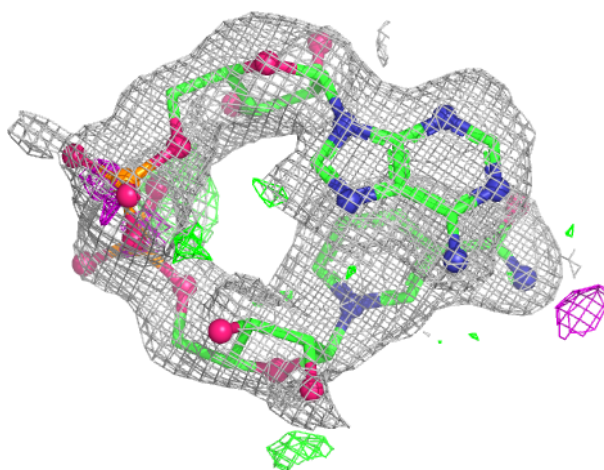
Electron density around NAI A 895:

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



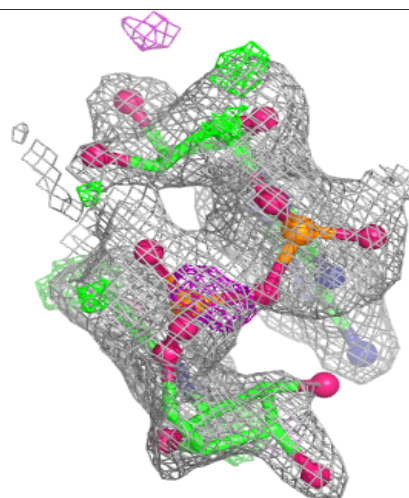
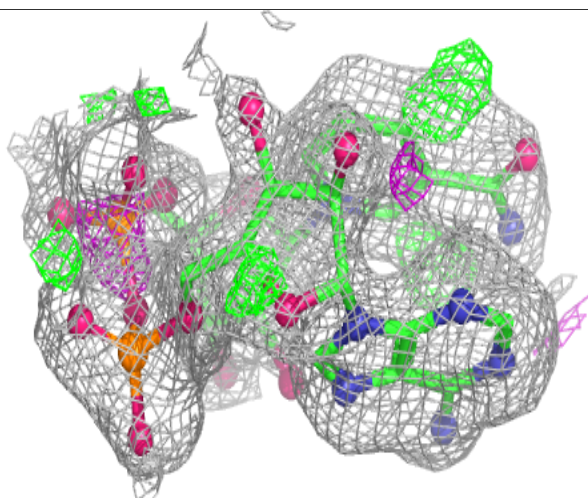
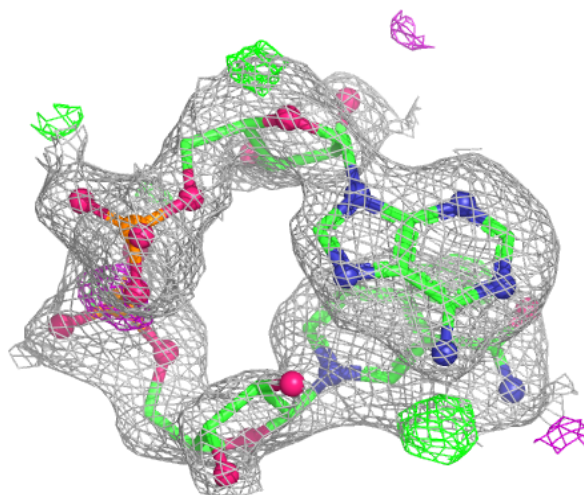
Electron density around NAI B 896:

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



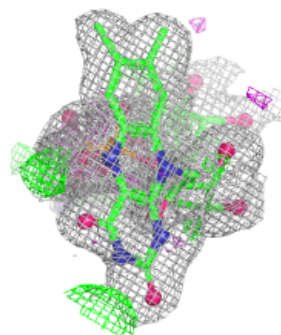
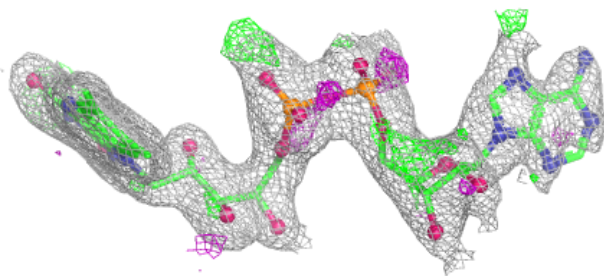
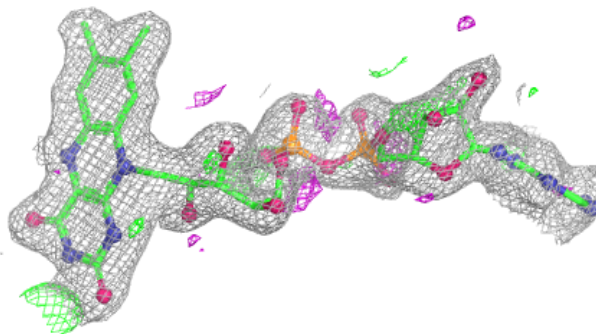
Electron density around NAI C 897:

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

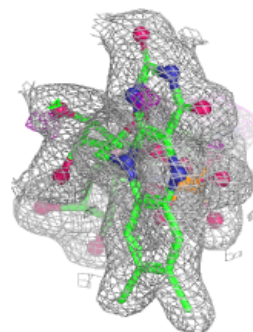
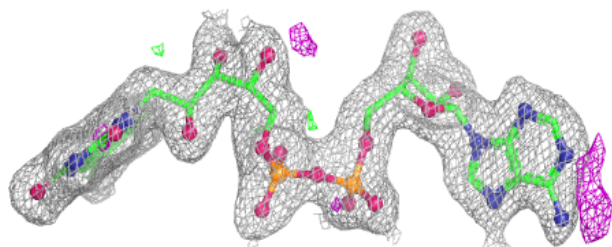
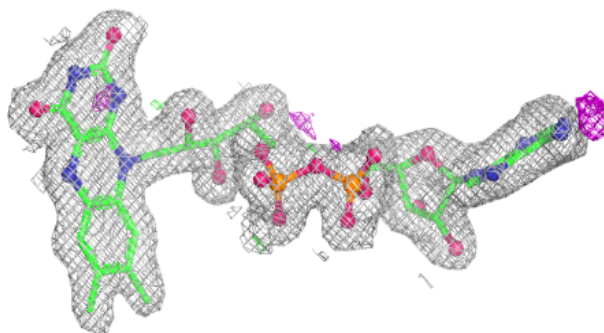


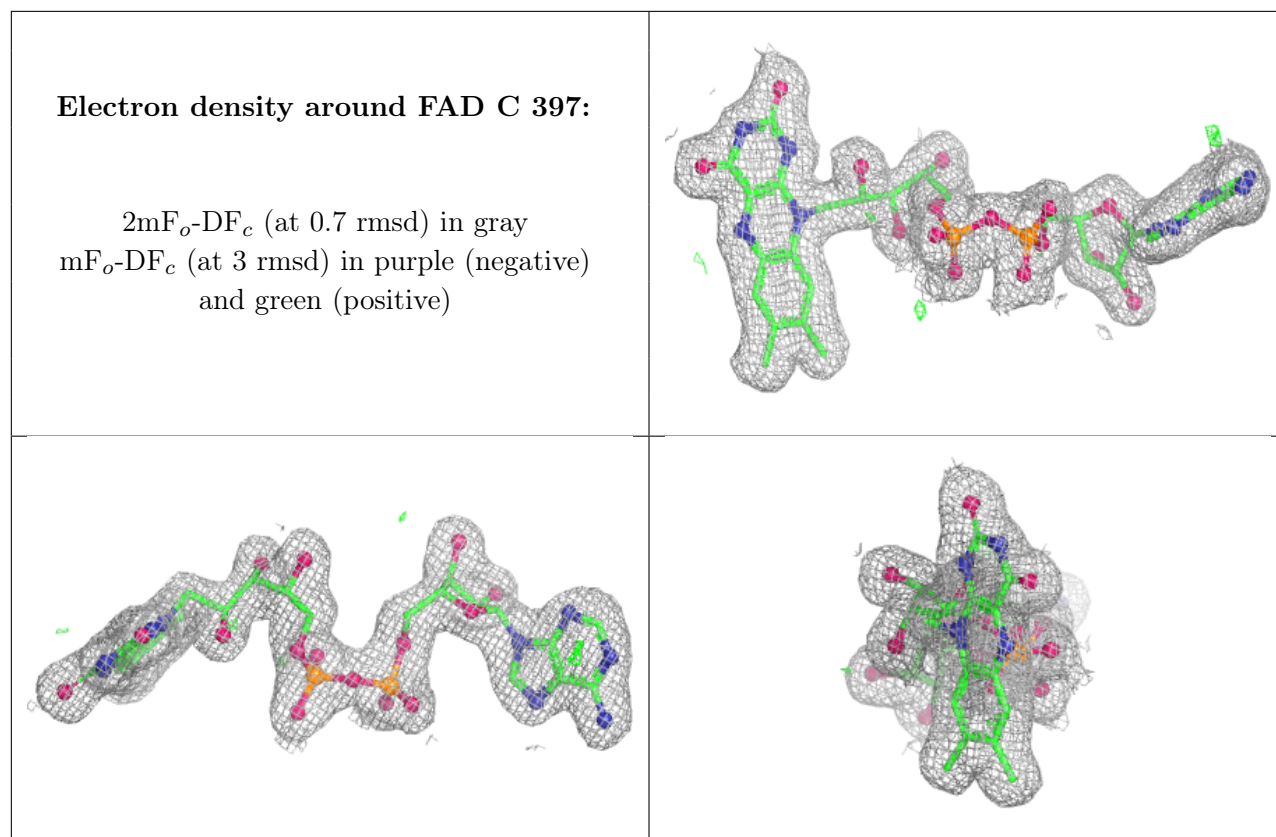
Electron density around FAD A 395:

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

**Electron density around FAD B 396:**

$2mF_o-DF_c$ (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.