



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:49 pm BST

PDB ID : 1ZP3
Title : E. coli Methylenetetrahydrofolate Reductase (oxidized)
Authors : Pejchal, R.; Sargeant, R.; Ludwig, M.L.
Deposited on : 2005-05-16
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

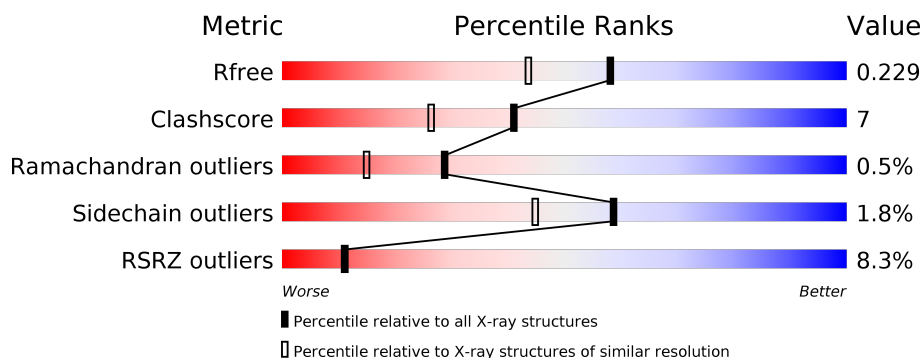
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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	
1	B	304	
1	C	304	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7110 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	284	Total	C	N	O	S	4	0	0
			2157	1368	376	402	11			
1	B	290	Total	C	N	O	S	4	0	0
			2242	1418	391	422	11			
1	C	267	Total	C	N	O	S	3	0	0
			2073	1315	363	384	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	304	HIS	-	EXPRESSION TAG	UNP P00394

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



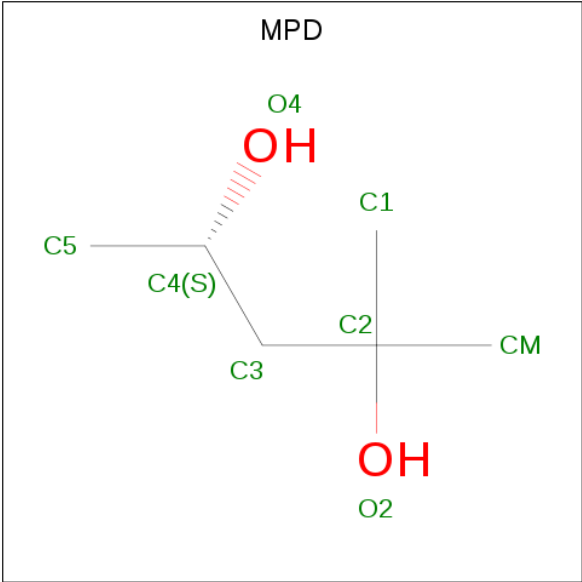
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	75	Total	O	0	0
			75	75		
5	B	186	Total	O	0	0
			186	186		
5	C	174	Total	O	0	0
			174	174		

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- 17% 74% 19% 7%
- MET SER PHE F4 H5 R9 L12 V10 Q20 Q21 Q22 P32 R33 E36 M37 E38 Q39 T40 L41 L42 N43 R47 Y60 G61 A62 N63 S64 G65 E66 R67 D68 R69 T70 H71 I74 I77 P87 T90 C91 I92 D93 A94 T95 P96 D97 E98 L99 R100 T101 I102 A103 R104 V107 M108 M109 G110 I111 R112 H113 I114 V115 A116 L117 D120 L121 P122 P140 G1Y SER G1Y LYS P140 G1U M130 Y131 A132 L135 V136 T137 L138 L139 K140 E141 L142 D143 A143 R149 G1U F145 V155 H156 P157 Q163 L169 K172 V173 A177 M178 R179 T182 Y182

- Chain B:
-
- 3% 81% 13% 5%
- MET SER F3 F4 H5 R9 L16 V19 D20 G21 R33 T34 S35 E36 I45 D46 R47 M63 E66 R67 K75 G76 I77 L89 T90 T95 P96 D97 H98 L99 R100 D105 Y106 W107 M108 M109 G110 I111 R112 L117 P122 F123 G124 SER GLY K127 R128

- Chain C:
-
- 3% 78% 9% 12%
- Horizontal bar chart for Chain C. The bar is divided into four segments: 3% green, 78% yellow, 9% orange, and 12% grey. Below the bar, a sequence of amino acids is listed, color-coded to match the segments: MET (grey), SER (grey), PHE (grey), HIS (grey), ALA (grey), SER (grey), GLN (grey), ARG (grey), ASP (grey), ALA (grey), LEU (grey), ASN (grey), GLN (grey), SER (grey), LEU (grey), ALA (grey), GLU (grey), VAL (grey), GLN (green), G21 (green), G22 (green), T34 (yellow), S35 (yellow), E36 (yellow), K54 (orange), F55 (orange), G61 (yellow), S64 (yellow), G65 (yellow), I92 (yellow), R118 (yellow), G119 (yellow), D120 (yellow), L121 (yellow), PRO (grey), PRO (grey), GLY (grey), SER (grey), GLY (grey), LYS (grey), PRO (grey), E129 (orange), A132 (yellow), T137 (yellow), L138 (yellow), E141 (yellow), D146 (yellow), V155 (yellow).

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.24Å 127.79Å 97.70Å 90.00° 121.55° 90.00°	Depositor
Resolution (Å)	19.91 – 1.85 19.91 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.91-1.85) 99.3 (19.91-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.237 0.206 , 0.229	Depositor DCC
R_{free} test set	9117 reflections (9.22%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7110	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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: MPD, SO4, 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	0.30	0/2200	0.51	0/2990
1	B	0.35	0/2289	0.58	1/3108 (0.0%)
1	C	0.36	0/2115	0.60	1/2866 (0.0%)
All	All	0.34	0/6604	0.56	2/8964 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	ASP	N-CA-C	-5.80	95.34	111.00
1	B	146	ASP	N-CA-C	-5.36	96.54	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2157	0	2071	44	0
1	B	2242	0	2168	27	0
1	C	2073	0	2027	24	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	31	0	0
3	B	53	0	31	0	0
3	C	53	0	31	0	0
4	A	8	0	13	0	0
4	B	8	0	13	1	0
4	C	8	0	14	1	0
5	A	75	0	0	1	0
5	B	186	0	0	6	0
5	C	174	0	0	3	0
All	All	7110	0	6399	92	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 7.

All (92) 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:100:ARG:HG2	1:A:138:LEU:HD11	1.42	0.99
1:B:179:ARG:NH1	5:B:677:HOH:O	2.20	0.74
1:A:100:ARG:CG	1:A:138:LEU:HD11	2.20	0.72
1:B:16:LEU:O	1:B:19:VAL:HG22	1.90	0.71
1:A:9:ARG:HD2	1:C:263:ILE:CD1	2.21	0.71
1:C:54:LYS:HE2	5:C:822:HOH:O	1.92	0.69
1:A:74:ILE:HG13	1:A:87:PRO:HB3	1.76	0.68
1:A:173:VAL:HA	1:A:177:ALA:HB3	1.74	0.67
1:A:9:ARG:HD2	1:C:263:ILE:HD12	1.76	0.67
1:C:231:ILE:HG23	1:C:235:MET:CE	2.26	0.66
1:B:63:ASN:OD1	1:B:122:PRO:HG3	1.96	0.65
1:B:149:VAL:HB	1:B:172:LYS:HE3	1.78	0.65
1:A:189:GLU:HG2	1:A:193:ARG:HH21	1.62	0.64
1:B:34:THR:OG1	1:B:36:GLU:HG2	1.98	0.63
1:C:222:LYS:O	1:C:226:MET:HG3	1.99	0.62
1:A:32:PRO:HB3	1:A:37:MET:HG3	1.82	0.61
1:B:36:GLU:H	1:B:36:GLU:CD	2.04	0.61
1:C:238:MET:HG3	1:C:252:VAL:HG11	1.83	0.60
1:A:143:ALA:HB3	1:A:145:PHE:CE1	2.37	0.60
1:B:200:SER:HB2	5:B:933:HOH:O	2.02	0.59
1:C:137:THR:O	1:C:141:GLU:HG3	2.02	0.59
1:A:247:GLU:H	1:A:247:GLU:CD	2.07	0.58
1:A:96:PRO:O	1:A:100:ARG:HG3	2.03	0.58
1:C:231:ILE:HG23	1:C:235:MET:HE2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ILE:HD13	1:B:77:ILE:HG12	1.85	0.58
1:A:90:THR:HA	1:A:117:LEU:O	2.04	0.57
1:A:121:LEU:HD12	1:A:121:LEU:O	2.04	0.57
1:B:238:MET:HA	1:B:238:MET:CE	2.34	0.57
1:A:95:THR:OG1	1:A:98:GLU:HB2	2.04	0.57
1:B:137:THR:O	1:B:141:GLU:HG3	2.05	0.57
1:C:34:THR:OG1	1:C:36:GLU:HG2	2.05	0.57
1:A:138:LEU:O	1:A:142:VAL:HG23	2.04	0.56
1:A:111:ILE:N	1:A:111:ILE:HD12	2.20	0.56
1:A:32:PRO:HD3	1:A:41:LEU:HD22	1.87	0.55
1:A:47:ARG:HH11	1:A:47:ARG:HG3	1.72	0.55
1:C:92:ILE:HG12	1:C:118:ARG:O	2.06	0.55
1:C:54:LYS:HD2	1:C:55:PHE:HD2	1.71	0.55
1:C:238:MET:HG3	1:C:252:VAL:CG1	2.36	0.55
1:B:67:ARG:HH11	1:B:67:ARG:HG2	1.73	0.54
1:C:231:ILE:HG23	1:C:235:MET:HE1	1.92	0.52
1:B:107:TRP:CZ3	1:B:112:ARG:HD2	2.45	0.52
1:B:90:THR:HA	1:B:117:LEU:O	2.10	0.52
1:B:238:MET:HA	1:B:238:MET:HE3	1.90	0.51
1:A:179:ARG:HH11	1:A:179:ARG:HG2	1.75	0.51
1:B:47:ARG:HH11	1:B:47:ARG:HG2	1.76	0.51
1:A:198:CYS:HB3	5:A:898:HOH:O	2.11	0.51
1:A:222:LYS:HG2	1:A:226:MET:CE	2.43	0.49
1:C:266:ARG:HG2	1:C:266:ARG:HH11	1.78	0.48
1:A:39:GLN:HG3	1:A:43:ASN:HD21	1.78	0.48
1:B:275:TYR:CD1	4:B:496:MPD:HM3	2.49	0.48
1:B:33:ARG:HD3	5:B:640:HOH:O	2.14	0.48
1:C:54:LYS:HD3	5:C:764:HOH:O	2.15	0.47
1:C:61:GLY:HA3	1:C:64:SER:OG	2.14	0.47
1:C:54:LYS:HD3	1:C:54:LYS:O	2.14	0.47
1:A:188:VAL:HG22	1:A:260:MET:HE2	1.97	0.46
1:A:193:ARG:HH11	1:A:193:ARG:HG2	1.79	0.46
1:A:132:ALA:HB3	1:A:172:LYS:HD3	1.98	0.46
1:A:227:THR:O	1:A:228:ASN:HB3	2.16	0.46
1:A:233:ALA:O	1:A:237:GLN:HG3	2.16	0.45
1:B:105:ASP:O	1:B:109:ASN:ND2	2.50	0.45
1:A:138:LEU:O	1:A:141:GLU:HG2	2.17	0.44
1:A:111:ILE:H	1:A:111:ILE:HD12	1.82	0.44
1:C:215:SER:HB3	1:C:282:MET:SD	2.56	0.44
1:B:138:LEU:HD23	1:B:138:LEU:C	2.37	0.44
1:A:222:LYS:HG2	1:A:226:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:MET:HG3	1:A:252:VAL:CG1	2.48	0.44
1:A:9:ARG:HH12	1:C:260:MET:HG2	1.83	0.43
1:C:277:LEU:HD21	4:C:497:MPD:H13	1.99	0.43
1:A:157:PRO:HG3	1:A:228:ASN:HB2	2.00	0.43
1:A:214:VAL:O	1:A:253:GLY:HA3	2.19	0.43
1:A:47:ARG:NH1	1:A:47:ARG:HG3	2.32	0.43
1:C:132:ALA:HB3	1:C:172:LYS:HD3	2.00	0.43
1:B:89:LEU:HD12	5:B:785:HOH:O	2.19	0.43
1:A:238:MET:HG3	1:A:252:VAL:HG11	1.99	0.43
1:A:135:LEU:O	1:A:139:LEU:HG	2.19	0.42
1:B:9:ARG:NH2	5:B:690:HOH:O	2.52	0.42
1:B:21:GLY:N	5:B:722:HOH:O	2.48	0.42
1:C:141:GLU:HB2	5:C:836:HOH:O	2.19	0.42
1:A:20:GLN:HA	1:A:291:GLY:HA3	2.00	0.42
1:B:33:ARG:HH12	1:B:66:GLU:CD	2.22	0.42
1:A:182:THR:CG2	1:A:207:ILE:HG22	2.50	0.42
1:A:199:VAL:HG13	1:A:200:SER:N	2.34	0.42
1:B:96:PRO:O	1:B:100:ARG:HG3	2.20	0.42
1:C:173:VAL:HA	1:C:177:ALA:HB3	2.02	0.42
1:A:247:GLU:N	1:A:247:GLU:CD	2.72	0.41
1:A:36:GLU:CD	1:A:36:GLU:H	2.24	0.41
1:B:173:VAL:HA	1:B:177:ALA:HB3	2.01	0.41
1:B:106:TYR:HB3	1:B:111:ILE:HB	2.03	0.41
1:B:95:THR:OG1	1:B:98:GLU:HG3	2.20	0.41
1:C:138:LEU:HD23	1:C:138:LEU:C	2.41	0.40
1:A:189:GLU:HG2	1:A:193:ARG:NH2	2.32	0.40
1:A:169:LEU:O	1:A:173:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	280/304 (92%)	271 (97%)	7 (2%)	2 (1%)	22	9
1	B	286/304 (94%)	282 (99%)	3 (1%)	1 (0%)	41	26
1	C	263/304 (86%)	259 (98%)	3 (1%)	1 (0%)	34	19
All	All	829/912 (91%)	812 (98%)	13 (2%)	4 (0%)	29	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	155	VAL
1	A	155	VAL
1	B	155	VAL
1	A	22	GLN

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	218/258 (84%)	213 (98%)	5 (2%)	50	34
1	B	234/258 (91%)	228 (97%)	6 (3%)	46	30
1	C	216/258 (84%)	215 (100%)	1 (0%)	88	86
All	All	668/774 (86%)	656 (98%)	12 (2%)	59	45

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ARG
1	A	120	ASP
1	A	179	ARG
1	A	193	ARG
1	A	195	ARG
1	B	36	GLU
1	B	67	ARG
1	B	75	LYS
1	B	206	GLU

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Mol	Chain	Res	Type
1	B	228	ASN
1	B	238	MET
1	C	54	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	39	GLN
1	A	43	ASN
1	A	168	ASN
1	B	168	ASN
1	C	228	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates 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	C	402	-	4,4,4	0.24	0	6,6,6	0.10	0
4	MPD	C	497	-	7,7,7	1.23	1 (14%)	9,10,10	0.39	0
3	FAD	A	395	-	51,58,58	1.91	10 (19%)	60,89,89	2.92	16 (26%)
2	SO4	A	400	-	4,4,4	0.25	0	6,6,6	0.04	0
2	SO4	B	399	-	4,4,4	0.26	0	6,6,6	0.08	0
3	FAD	B	396	-	51,58,58	1.85	12 (23%)	60,89,89	3.00	18 (30%)
4	MPD	A	495	-	7,7,7	1.32	1 (14%)	9,10,10	0.41	0
3	FAD	C	397	-	51,58,58	1.75	9 (17%)	60,89,89	2.68	11 (18%)
4	MPD	B	496	-	7,7,7	1.27	1 (14%)	9,10,10	0.40	0
2	SO4	A	401	-	4,4,4	0.28	0	6,6,6	0.08	0

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	MPD	C	497	-	-	0/5/5/5	-
3	FAD	A	395	-	-	7/30/50/50	0/6/6/6
3	FAD	B	396	-	-	2/30/50/50	0/6/6/6
4	MPD	A	495	-	-	0/5/5/5	-
3	FAD	C	397	-	-	1/30/50/50	0/6/6/6
4	MPD	B	496	-	-	3/5/5/5	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	395	FAD	C9A-N10	7.58	1.48	1.38
3	B	396	FAD	C9A-N10	6.36	1.47	1.38
3	C	397	FAD	C4X-N5	5.61	1.41	1.33
3	A	395	FAD	C4X-N5	5.17	1.40	1.33
3	C	397	FAD	C9A-N10	5.01	1.45	1.38
3	B	396	FAD	C4X-N5	4.95	1.40	1.33
3	C	397	FAD	C4-N3	4.35	1.40	1.33
3	A	395	FAD	O4B-C1B	3.79	1.46	1.41
3	A	395	FAD	C4-N3	3.62	1.39	1.33
3	B	396	FAD	C4-N3	3.61	1.39	1.33
3	A	395	FAD	C10-N1	3.31	1.37	1.33
4	A	495	MPD	O2-C2	-3.24	1.36	1.44
4	B	496	MPD	O2-C2	-3.15	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	396	FAD	C10-N1	3.13	1.37	1.33
3	B	396	FAD	C5X-N5	3.09	1.40	1.35
4	C	497	MPD	O2-C2	-3.07	1.36	1.44
3	A	395	FAD	C8-C7	2.92	1.48	1.40
3	B	396	FAD	C8-C7	2.84	1.48	1.40
3	B	396	FAD	C9-C9A	2.82	1.46	1.40
3	C	397	FAD	C9-C9A	2.69	1.46	1.40
3	B	396	FAD	O4B-C1B	2.61	1.44	1.41
3	B	396	FAD	C6-C5X	2.56	1.45	1.41
3	C	397	FAD	C10-N1	2.49	1.36	1.33
3	C	397	FAD	C5X-N5	2.41	1.39	1.35
3	A	395	FAD	C5'-C4'	2.25	1.55	1.51
3	B	396	FAD	C8M-C8	2.20	1.55	1.51
3	C	397	FAD	C8M-C8	2.19	1.55	1.51
3	B	396	FAD	C2-N1	-2.16	1.33	1.38
3	A	395	FAD	C2-N1	-2.16	1.33	1.38
3	B	396	FAD	C7M-C7	2.15	1.55	1.51
3	A	395	FAD	C9-C9A	2.12	1.45	1.40
3	C	397	FAD	C8A-N7A	-2.12	1.30	1.34
3	A	395	FAD	C8A-N7A	-2.08	1.31	1.34
3	C	397	FAD	C2-N1	-2.07	1.34	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	396	FAD	C4-N3-C2	16.18	128.81	115.14
3	A	395	FAD	C4-N3-C2	14.66	127.52	115.14
3	C	397	FAD	C4-N3-C2	13.85	126.84	115.14
3	B	396	FAD	C10-C4X-N5	8.09	126.85	121.26
3	A	395	FAD	C10-C4X-N5	8.07	126.84	121.26
3	B	396	FAD	C4X-C4-N3	-6.52	114.51	123.43
3	C	397	FAD	C4-C4X-C10	-6.52	115.63	119.95
3	C	397	FAD	C10-C4X-N5	6.06	125.45	121.26
3	A	395	FAD	C4X-C4-N3	-5.89	115.38	123.43
3	C	397	FAD	C4X-C4-N3	-5.87	115.41	123.43
3	B	396	FAD	C4-C4X-C10	-5.76	116.14	119.95
3	A	395	FAD	C4-C4X-C10	-5.51	116.30	119.95
3	C	397	FAD	C4X-C10-N10	-4.64	115.53	120.30
3	A	395	FAD	C4X-C10-N10	-4.58	115.59	120.30
3	A	395	FAD	C5X-C9A-N10	-4.53	114.43	117.72
3	B	396	FAD	C4X-C10-N10	-4.40	115.78	120.30
3	C	397	FAD	C5X-C9A-N10	-4.04	114.79	117.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	395	FAD	C5'-C4'-C3'	3.98	119.89	112.20
3	B	396	FAD	C1'-N10-C9A	3.85	121.32	118.29
3	B	396	FAD	C5X-C9A-N10	-3.51	115.17	117.72
3	C	397	FAD	C1'-N10-C9A	3.44	121.00	118.29
3	A	395	FAD	C6-C5X-N5	-3.42	115.28	119.05
3	C	397	FAD	O5'-C5'-C4'	3.21	117.94	109.36
3	A	395	FAD	C8M-C8-C7	3.10	127.08	120.74
3	B	396	FAD	O5'-C5'-C4'	2.85	116.97	109.36
3	A	395	FAD	O2'-C2'-C3'	2.66	115.57	109.10
3	A	395	FAD	C4'-C3'-C2'	2.55	118.67	113.36
3	B	396	FAD	C5'-C4'-C3'	2.50	117.04	112.20
3	A	395	FAD	C8M-C8-C9	-2.45	114.49	120.34
3	B	396	FAD	O5B-C5B-C4B	2.44	117.40	108.99
3	A	395	FAD	C9A-C5X-N5	2.42	126.15	122.36
3	A	395	FAD	C1'-N10-C9A	2.23	120.05	118.29
3	B	396	FAD	O2B-C2B-C1B	2.20	119.00	110.85
3	C	397	FAD	C6-C5X-N5	-2.16	116.67	119.05
3	C	397	FAD	C1B-N9A-C4A	-2.15	122.86	126.64
3	C	397	FAD	C5A-C6A-N6A	2.13	123.59	120.35
3	B	396	FAD	C8M-C8-C7	2.11	125.06	120.74
3	B	396	FAD	C6-C5X-N5	-2.10	116.73	119.05
3	B	396	FAD	O3'-C3'-C4'	2.10	113.88	108.81
3	B	396	FAD	C8M-C8-C9	-2.09	115.35	120.34
3	B	396	FAD	C1B-N9A-C4A	-2.06	123.02	126.64
3	B	396	FAD	O2P-P-O1P	2.05	122.38	112.24
3	A	395	FAD	C7M-C7-C6	-2.04	115.46	120.34
3	A	395	FAD	O5B-C5B-C4B	2.02	115.95	108.99
3	B	396	FAD	O2'-C2'-C3'	2.01	113.97	109.10

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	395	FAD	O2'-C2'-C3'-C4'
3	B	396	FAD	O2'-C2'-C3'-C4'
3	A	395	FAD	O4'-C4'-C5'-O5'
3	A	395	FAD	C5B-O5B-PA-O1A
4	B	496	MPD	C1-C2-C3-C4
4	B	496	MPD	CM-C2-C3-C4
3	C	397	FAD	O2'-C2'-C3'-C4'
3	A	395	FAD	C2'-C3'-C4'-C5'
4	B	496	MPD	O2-C2-C3-C4

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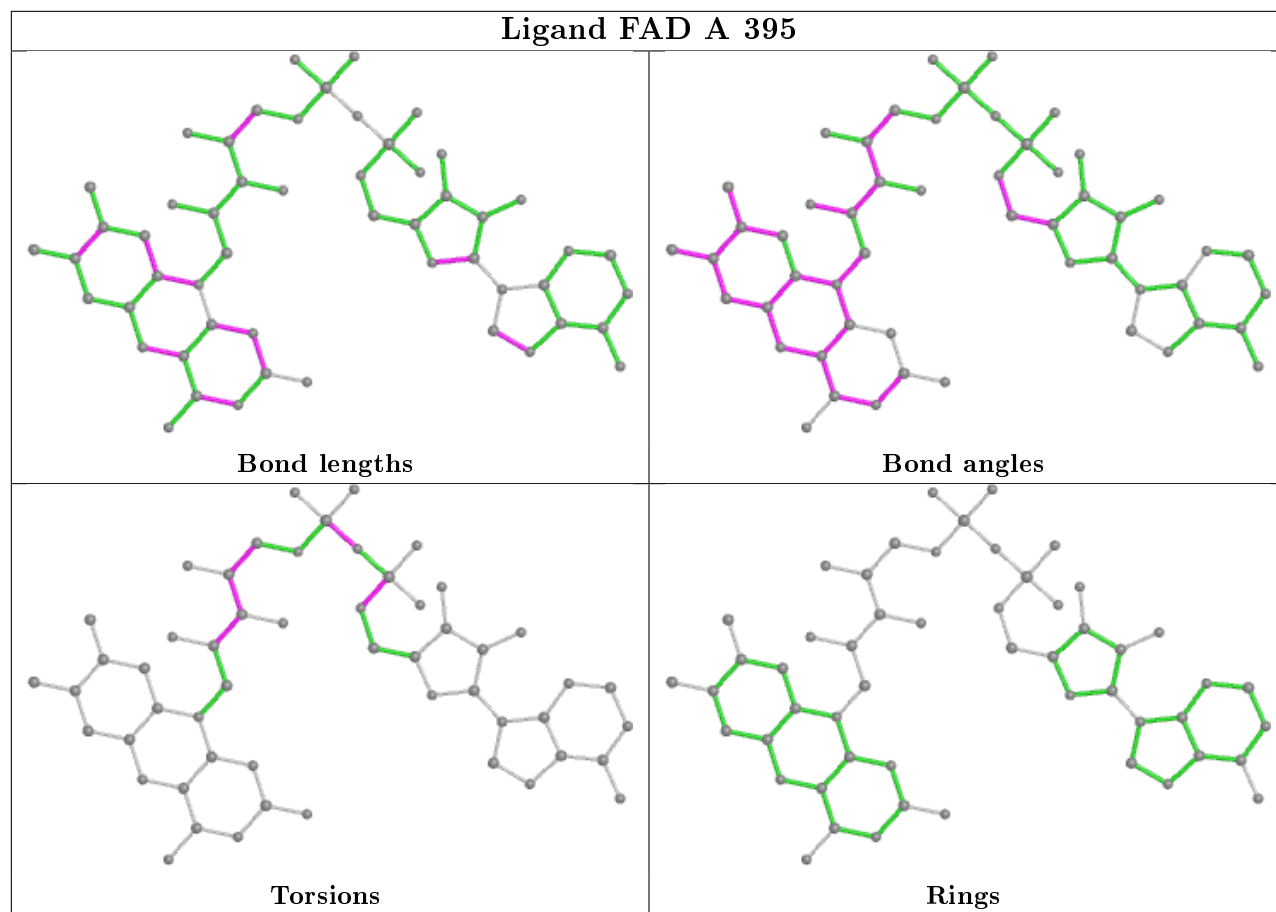
Mol	Chain	Res	Type	Atoms
3	A	395	FAD	C5B-O5B-PA-O3P
3	A	395	FAD	O3'-C3'-C4'-C5'
3	A	395	FAD	PA-O3P-P-O2P
3	B	396	FAD	P-O3P-PA-O2A

There are no ring outliers.

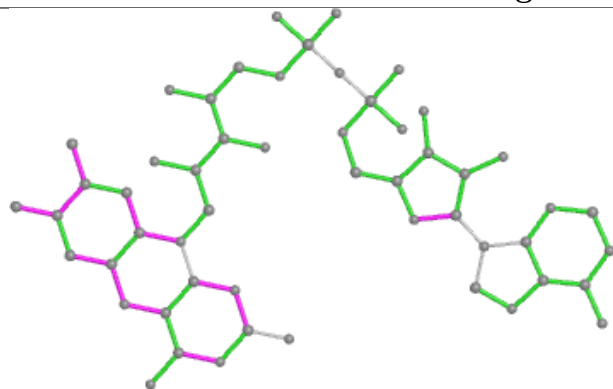
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	497	MPD	1	0
4	B	496	MPD	1	0

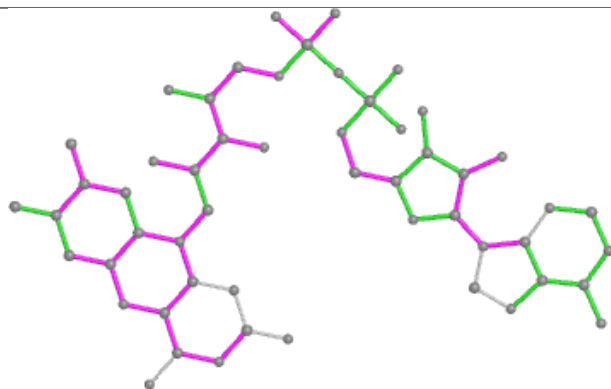
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



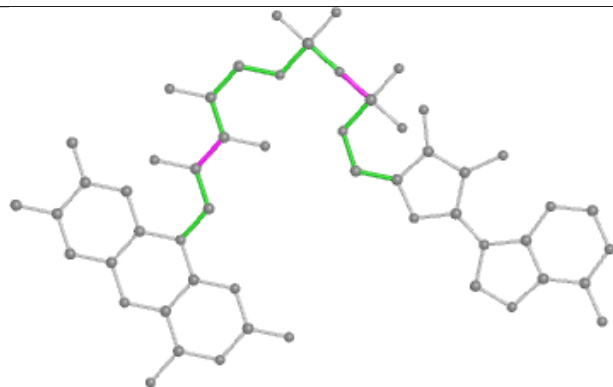
Ligand FAD B 396



Bond lengths



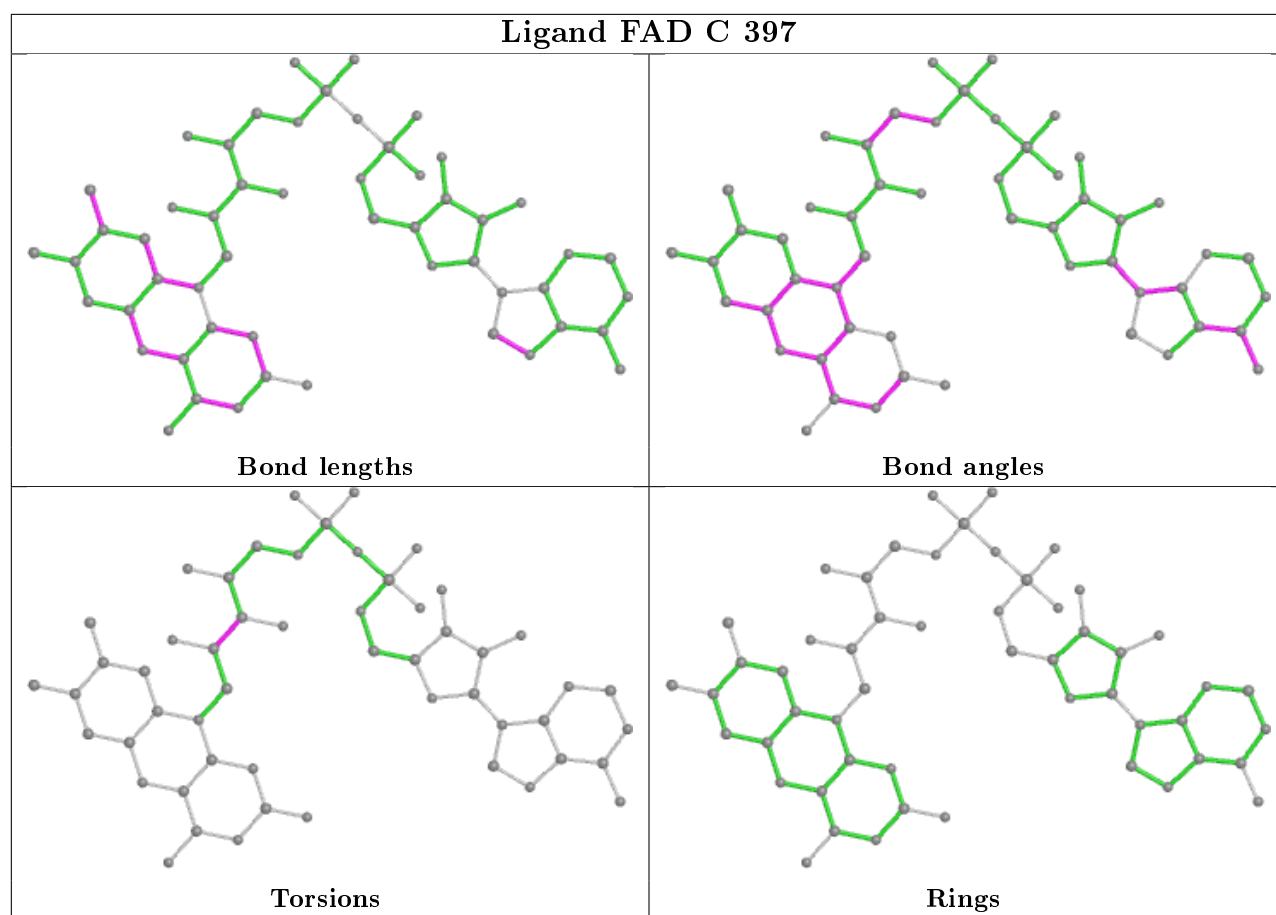
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	284/304 (93%)	1.05	53 (18%) 1 1	18, 41, 64, 73	1 (0%)
1	B	290/304 (95%)	0.05	9 (3%) 49 47	13, 23, 40, 56	1 (0%)
1	C	267/304 (87%)	-0.04	8 (2%) 50 48	14, 21, 35, 53	1 (0%)
All	All	841/912 (92%)	0.36	70 (8%) 11 11	13, 27, 57, 73	3 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	GLY	8.5
1	A	121	LEU	8.4
1	C	121	LEU	7.7
1	C	21	GLY	6.0
1	A	65	GLY	5.7
1	A	122	PRO	5.6
1	B	123	PRO	5.3
1	A	4	PHE	4.9
1	A	5	HIS	4.7
1	A	93	ASP	4.7
1	B	21	GLY	4.3
1	A	92	ILE	4.2
1	B	226	MET	3.9
1	A	109	ASN	3.9
1	A	226	MET	3.6
1	A	107	TRP	3.6
1	A	145	PHE	3.6
1	A	62	ALA	3.5
1	A	63	ASN	3.4
1	A	144	ASP	3.4
1	A	120	ASP	3.4
1	A	97	ASP	3.3
1	A	104	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	266	ARG	3.1
1	A	94	ALA	3.1
1	A	68	ASP	3.0
1	A	189	GLU	2.9
1	B	127	LYS	2.7
1	A	12	LEU	2.7
1	B	129	GLU	2.7
1	A	179	ARG	2.7
1	A	112	ARG	2.7
1	C	92	ILE	2.6
1	A	19	VAL	2.6
1	A	116	ALA	2.6
1	A	71	HIS	2.6
1	A	115	VAL	2.6
1	A	132	ALA	2.6
1	C	65	GLY	2.6
1	A	39	GLN	2.6
1	A	66	GLU	2.6
1	A	136	VAL	2.5
1	A	60	TYR	2.5
1	B	122	PRO	2.5
1	C	120	ASP	2.4
1	A	67	ARG	2.4
1	A	222	LYS	2.4
1	A	101	THR	2.4
1	A	33	ARG	2.4
1	B	124	GLY	2.4
1	A	99	LEU	2.3
1	A	111	ILE	2.3
1	B	5	HIS	2.3
1	A	143	ALA	2.3
1	A	95	THR	2.2
1	A	139	LEU	2.2
1	A	102	ILE	2.2
1	A	70	THR	2.2
1	A	77	ILE	2.2
1	A	163	GLN	2.2
1	A	114	ILE	2.1
1	C	22	GLN	2.1
1	A	131	TYR	2.1
1	A	130	MET	2.1
1	A	135	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	226	MET	2.1
1	A	117	LEU	2.1
1	A	225	ASP	2.1
1	B	19	VAL	2.1
1	A	141	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

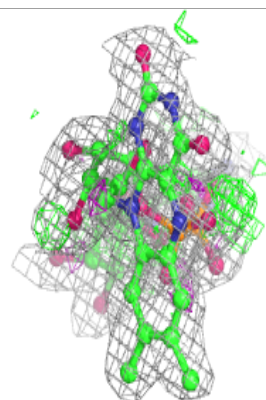
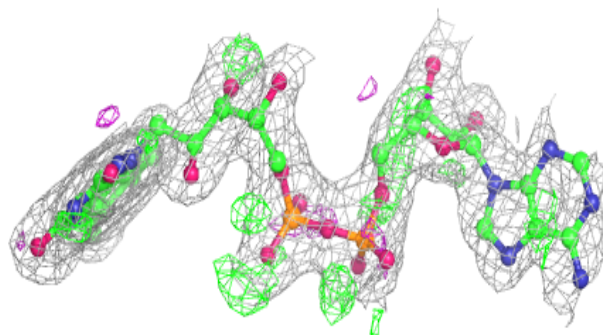
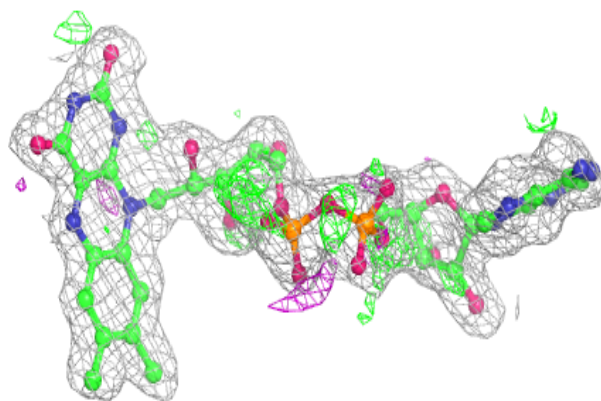
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MPD	B	496	8/8	0.81	0.28	31,32,33,34	8
3	FAD	A	395	53/53	0.82	0.16	30,37,55,55	0
4	MPD	A	495	8/8	0.83	0.23	36,38,39,40	8
4	MPD	C	497	8/8	0.87	0.19	31,33,34,34	8
2	SO4	A	401	5/5	0.93	0.16	48,48,49,49	0
2	SO4	A	400	5/5	0.95	0.12	56,56,57,57	5
3	FAD	C	397	53/53	0.96	0.08	15,18,28,31	0
3	FAD	B	396	53/53	0.96	0.08	12,18,28,30	0
2	SO4	B	399	5/5	0.96	0.11	28,30,30,30	5
2	SO4	C	402	5/5	0.97	0.12	30,31,31,34	5

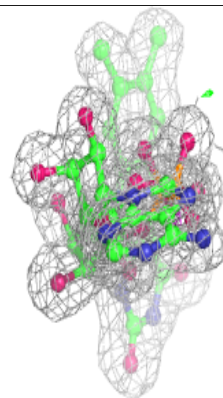
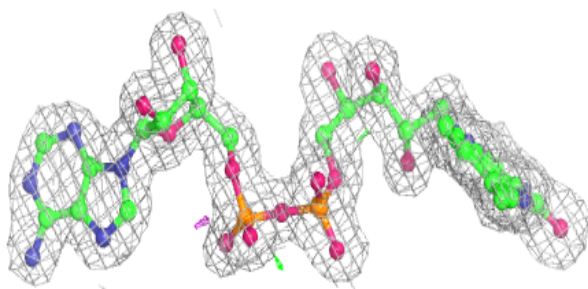
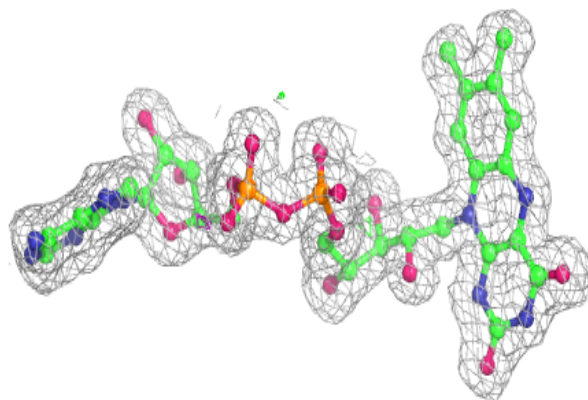
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD 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)

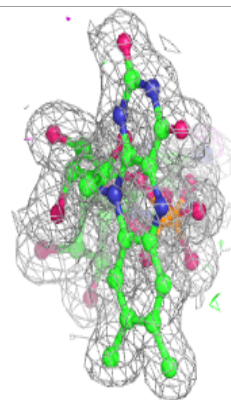
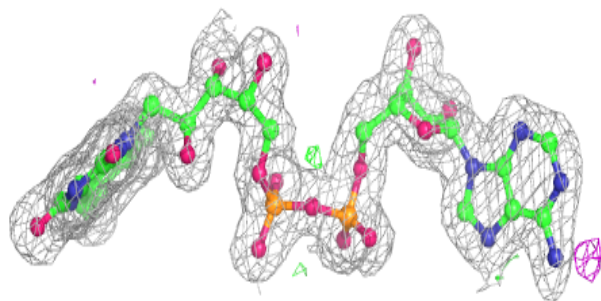
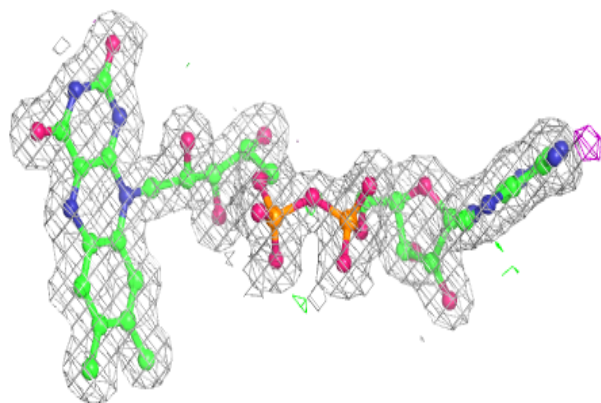
**Electron density around FAD C 397:**

$2mF_o-DF_c$ (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.