wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 10:58 am BST

PDB ID	:	1EA0
Title	:	Alpha subunit of A. brasilense glutamate synthase
Authors	:	Binda, C.; Bossi, R.T.; Vanoni, M.A.; Mattevi, A.
Deposited on	:	2000-11-02
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

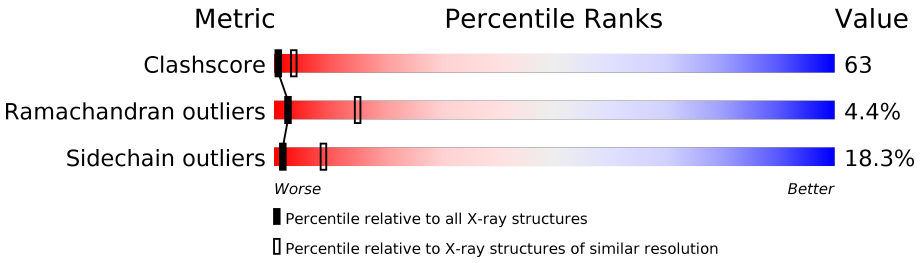
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1479	26% 50% 19%
1	B	1479	31% 47% 16%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OMT	A	2473	-	X	-	-
5	F3S	A	2476	-	-	X	-
5	F3S	B	2476	-	-	X	-

2 Entry composition (i)

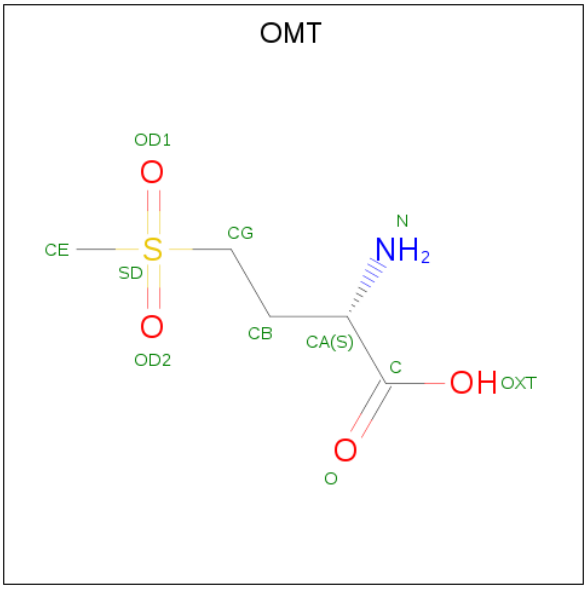
There are 5 unique types of molecules in this entry. The entry contains 22478 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN.

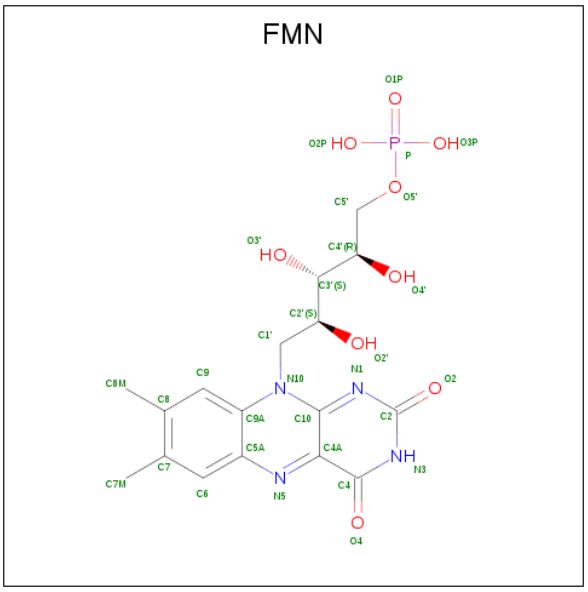
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1452	Total	C	N	O	S	0	0	0
			11180	7018	2005	2098	59			
1	B	1452	Total	C	N	O	S	0	0	0
			11180	7018	2005	2098	59			

- Molecule 2 is S-DIOXYMETHIONINE (three-letter code: OMT) (formula: $C_5H_{11}NO_4S$).



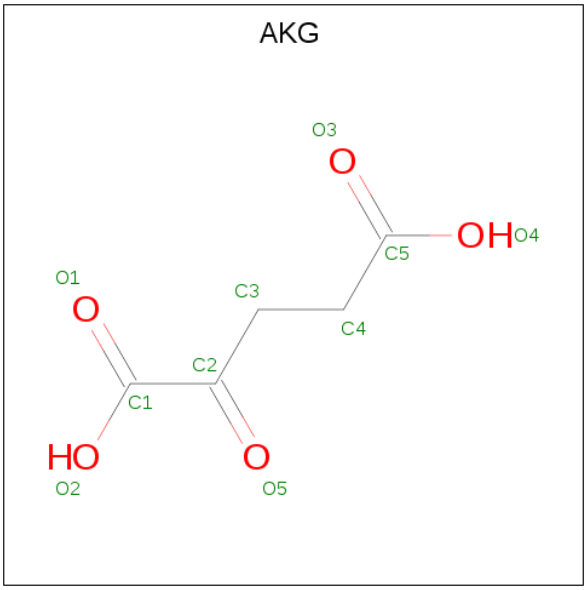
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			11	5	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			11	5	1	4	1		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



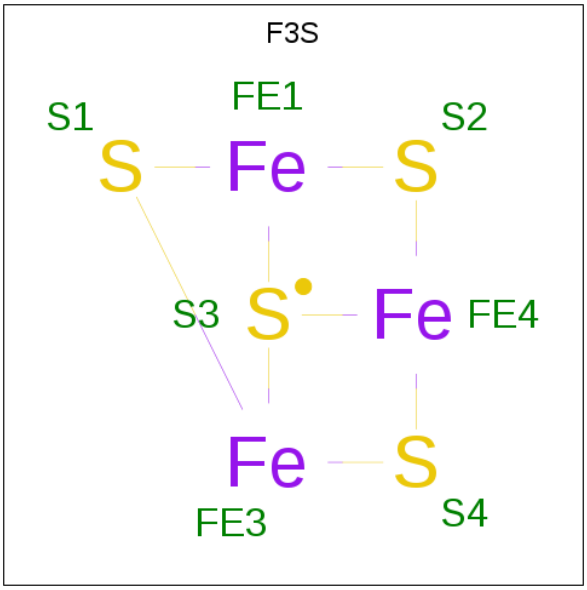
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			10	5	5			
4	B	1	Total	C	O		0	0
			10	5	5			

- Molecule 5 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe S 7 3 4	0	0
5	B	1	Total Fe S 7 3 4	0	0

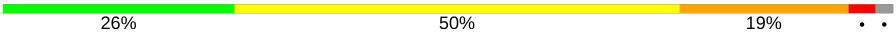
3 Residue-property plots (i)

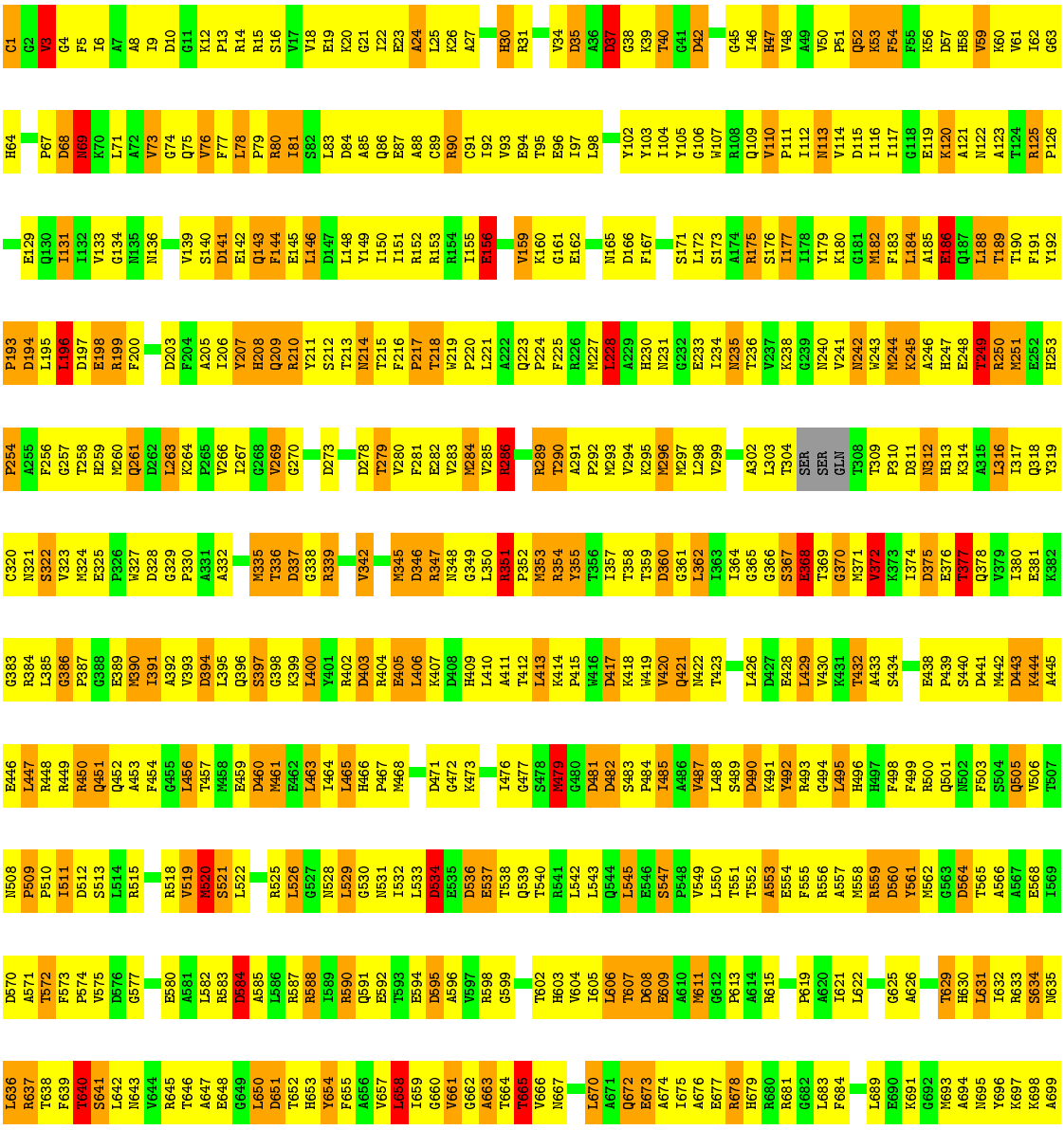
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

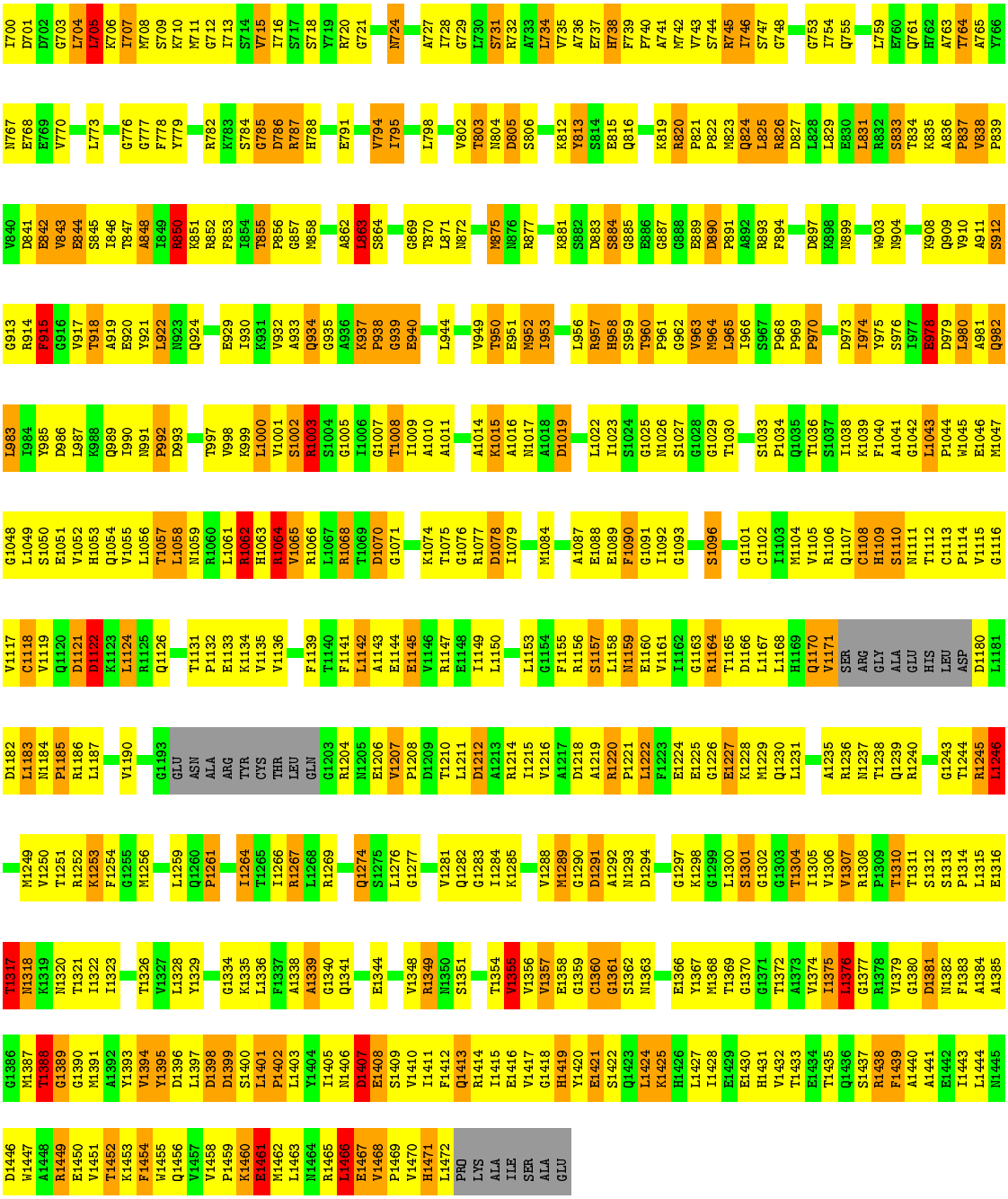
Note EDS was not executed.

- Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN

Chain A:

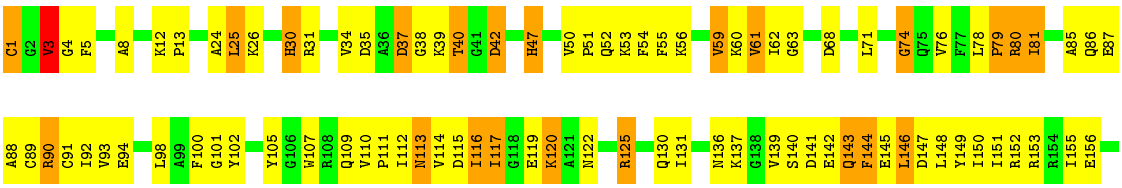


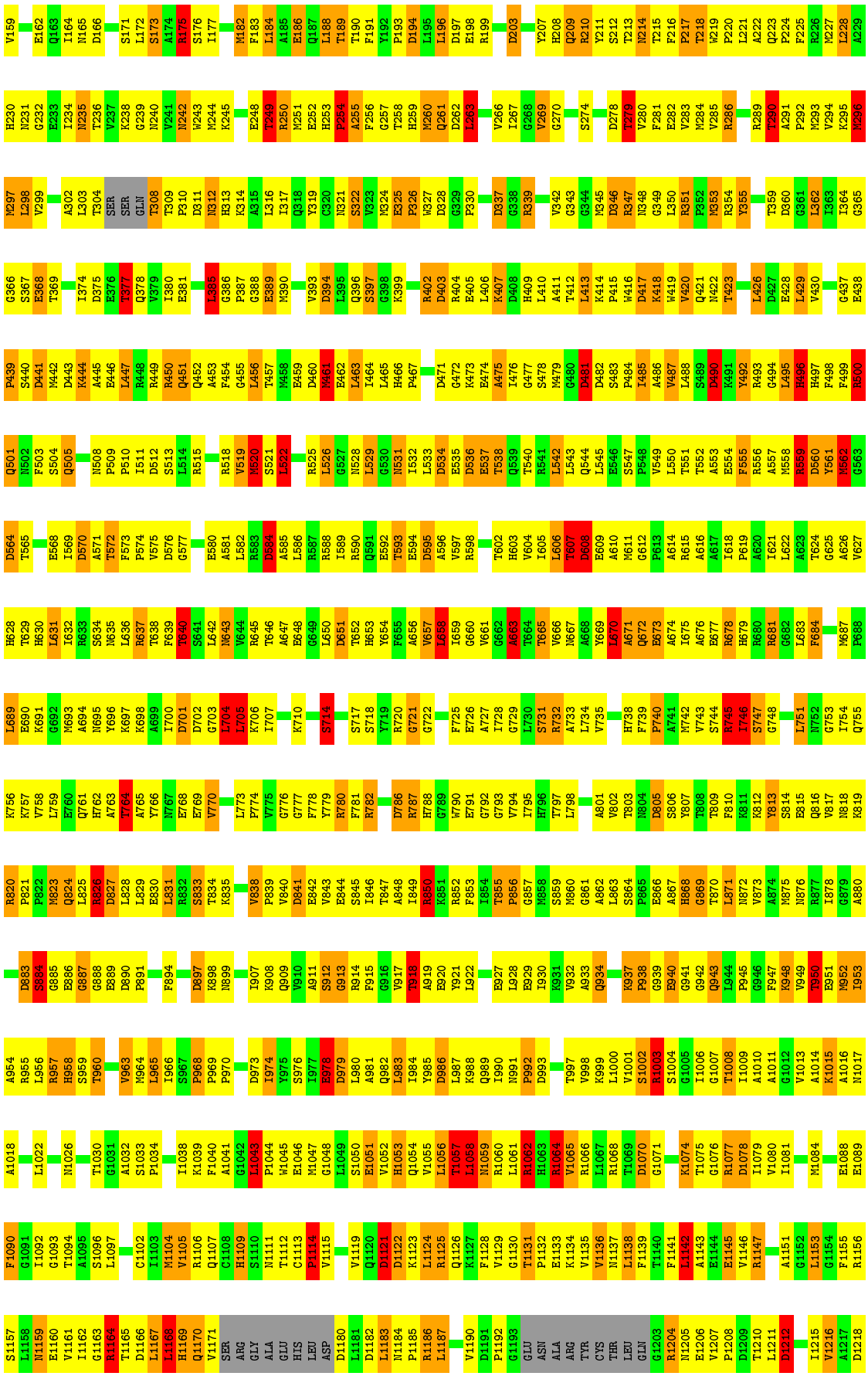


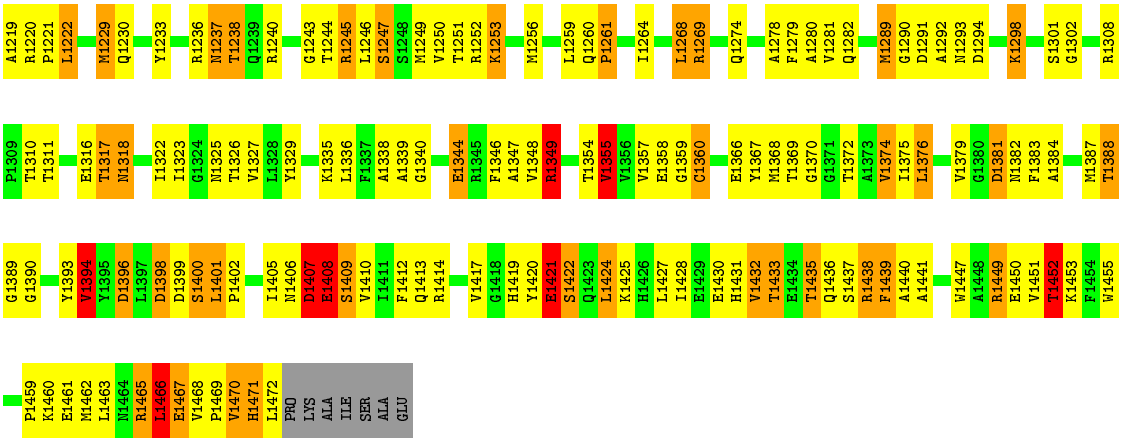


• Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN

Chain B:






A1219 R1220 P1221 L1222 M1229 Q1230 Y1233 R1236 N1237 T1238 Q1239 R1240 G1243 T1244 R1245 L1246 S1247 S1248 M1249 V1250 T1251 R1252 K1253 M1256 L1259 Q1260 P1261 I1264 L1268 R1269 Q1274 A1278 F1279 A1280 V1281 Q1282 M1289 G1290 D1291 A1292 N1293 D1294 K1298 S1301 G1302 R1308
P1309 T1310 T1311 E1316 T1317 N1318 I1322 I1323 G1324 N1325 T1326 V1327 L1328 Y1329 K1335 L1336 F1337 A1338 A1339 G1340 E1344 R1345 F1346 A1347 V1348 R1349 T1354 V1355 V1356 V1357 E1358 G1359 C1360 E1366 Y1367 M1368 T1369 G1370 G1371 T1372 A1373 V1374 I1375 L1376 V1379 G1380 D1381 N1382 F1383 A1384 M1387 T1388
G1389 G1390 Y1393 V1394 Y1395 D1396 L1397 D1398 D1399 S1400 L1401 P1402 I1405 N1406 D1407 E1408 S1409 V1410 I1411 F1412 Q1413 R1414 V1417 G1418 H1419 Y1420 E1421 S1422 Q1423 L1424 K1425 H1426 L1427 I1428 E1429 E1430 H1431 V1432 T1433 E1434 T1435 Q1436 S1437 R1438 F1439 A1440 A1441 W1447 A1448 R1449 E1450 V1451 T1452 K1453 F1454 W1455
P1459 K1460 E1461 M1462 L1463 N1464 R1465 L1466 E1467 V1468 P1469 V1470 H1471 L1472 PRO LYS ALA ILE SER ALA GLU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	233.61Å 233.61Å 305.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	98.6 (20.00-3.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.256 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22478	wwPDB-VP
Average B, all atoms (Å^2)	57.0	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: FMN, F3S, AKG, OMT

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	1.06	7/11383 (0.1%)	1.58	198/15390 (1.3%)
1	B	1.10	7/11383 (0.1%)	1.58	192/15390 (1.2%)
All	All	1.08	14/22766 (0.1%)	1.58	390/30780 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	0	2
All	All	1	4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	838	VAL	CA-CB	-7.71	1.38	1.54
1	A	746	ILE	CA-CB	-7.47	1.37	1.54
1	A	848	ALA	CA-CB	-6.51	1.38	1.52
1	A	1065	VAL	CB-CG2	-6.15	1.40	1.52
1	A	3	VAL	CA-CB	-5.67	1.42	1.54

The worst 5 of 390 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1062	ARG	NE-CZ-NH1	-12.86	113.87	120.30
1	A	608	ASP	CB-CG-OD2	12.18	129.26	118.30
1	A	141	ASP	CB-CG-OD2	11.98	129.08	118.30
1	B	888	GLY	N-CA-C	-11.68	83.89	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	890	ASP	CB-CG-OD1	11.31	128.48	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	915	PHE	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1002	SER	Mainchain
1	A	325	GLU	Mainchain
1	B	1168	LEU	Mainchain
1	B	725	PHE	Mainchain

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	11180	0	11210	1498	0
1	B	11180	0	11212	1318	0
2	A	11	0	10	2	0
2	B	11	0	10	1	0
3	A	31	0	19	4	0
3	B	31	0	19	6	0
4	A	10	0	4	0	0
4	B	10	0	4	2	0
5	A	7	0	0	2	0
5	B	7	0	0	3	0
All	All	22478	0	22488	2814	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 63.

The worst 5 of 2814 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:B:182:MET:CE	1:B:217:PRO:HB2	1.30	1.59
1:A:182:MET:HE3	1:A:217:PRO:CB	1.34	1.57
1:B:1449:ARG:CB	1:B:1449:ARG:HH11	0.97	1.56
1:B:182:MET:HE3	1:B:217:PRO:CB	1.09	1.54
1:A:182:MET:CE	1:A:217:PRO:HB2	1.45	1.47

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	1444/1479 (98%)	1152 (80%)	227 (16%)	65 (4%)	2 14
1	B	1444/1479 (98%)	1170 (81%)	211 (15%)	63 (4%)	2 15
All	All	2888/2958 (98%)	2322 (80%)	438 (15%)	128 (4%)	2 15

5 of 128 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	444	LYS
1	A	451	GLN
1	A	705	LEU
1	A	712	GLY

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	A	1184/1206 (98%)	970 (82%)	214 (18%)	1 9
1	B	1184/1206 (98%)	965 (82%)	219 (18%)	1 8
All	All	2368/2412 (98%)	1935 (82%)	433 (18%)	1 9

5 of 433 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1381	ASP
1	B	215	THR
1	B	1246	LEU
1	A	1413	GLN
1	B	40	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1320	ASN
1	B	113	ASN
1	B	1274	GLN
1	A	1363	ASN
1	B	30	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	AKG	B	2475	-	3,9,9	5.21	2 (66%)	4,11,11	4.04	2 (50%)
4	AKG	A	2475	-	3,9,9	4.84	2 (66%)	4,11,11	3.45	2 (50%)
5	F3S	B	2476	1	0,9,9	0.00	-	-		
3	FMN	B	2474	-	31,33,33	1.49	3 (9%)	40,50,50	3.22	19 (47%)
2	OMT	A	2473	-	6,10,10	4.94	4 (66%)	6,14,14	5.93	5 (83%)
3	FMN	A	2474	-	31,33,33	1.56	6 (19%)	40,50,50	3.12	20 (50%)
5	F3S	A	2476	1	0,9,9	0.00	-	-		
2	OMT	B	2473	-	6,10,10	4.89	4 (66%)	6,14,14	7.72	4 (66%)

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	AKG	B	2475	-	-	1/3/9/9	-
4	AKG	A	2475	-	-	0/3/9/9	-
5	F3S	B	2476	1	-	-	0/3/3/3
3	FMN	B	2474	-	-	5/18/18/18	0/3/3/3
2	OMT	A	2473	-	-	5/6/10/10	-
3	FMN	A	2474	-	-	7/18/18/18	0/3/3/3
5	F3S	A	2476	1	-	-	0/3/3/3
2	OMT	B	2473	-	-	5/6/10/10	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2475	AKG	O5-C2	8.69	1.36	1.22
4	A	2475	AKG	O5-C2	8.07	1.35	1.22
2	A	2473	OMT	CB-CG	-6.99	1.45	1.52
2	B	2473	OMT	CG-SD	-6.88	1.69	1.78
2	A	2473	OMT	CG-SD	-6.69	1.69	1.78

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2473	OMT	OD2-SD-CG	-16.70	96.65	108.34
2	A	2473	OMT	OD2-SD-CE	-11.66	97.19	108.91
3	B	2474	FMN	C1'-N10-C10	8.14	125.70	118.41
3	A	2474	FMN	O5'-P-O1P	-7.87	84.41	106.47
3	B	2474	FMN	C1'-N10-C9A	-7.66	112.26	118.29

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2474	FMN	C2'-C3'-C4'-O4'
3	B	2474	FMN	O3'-C3'-C4'-O4'
2	A	2473	OMT	C-CA-CB-CG
2	A	2473	OMT	CB-CG-SD-OD1
2	A	2473	OMT	CB-CG-SD-OD2

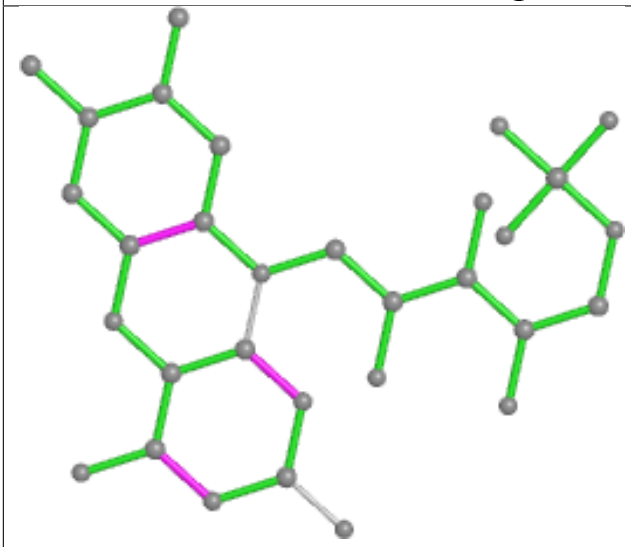
There are no ring outliers.

7 monomers are involved in 20 short contacts:

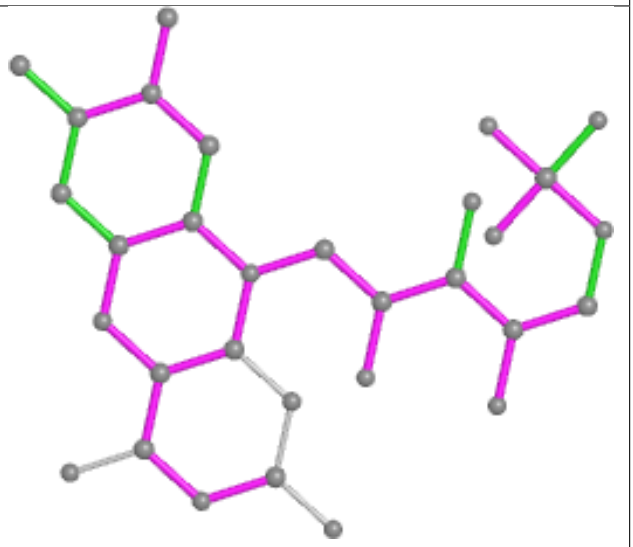
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2475	AKG	2	0
5	B	2476	F3S	3	0
3	B	2474	FMN	6	0
2	A	2473	OMT	2	0
3	A	2474	FMN	4	0
5	A	2476	F3S	2	0
2	B	2473	OMT	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

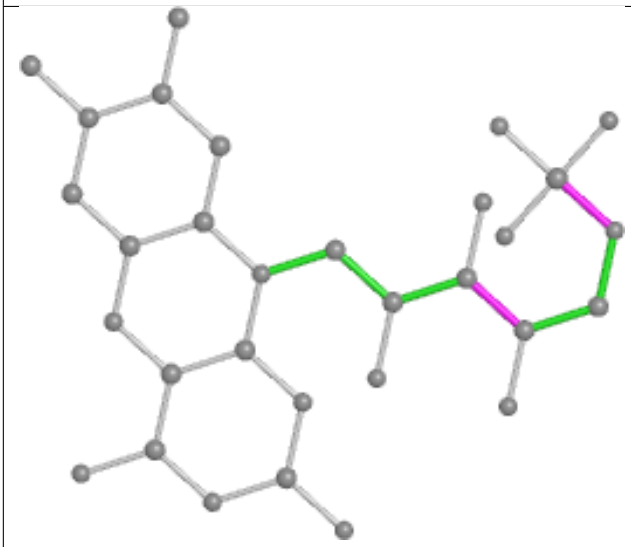
Ligand FMN B 2474



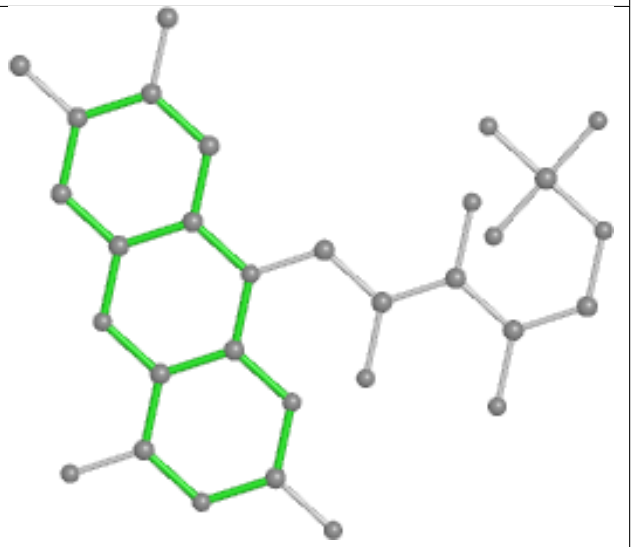
Bond lengths



Bond angles

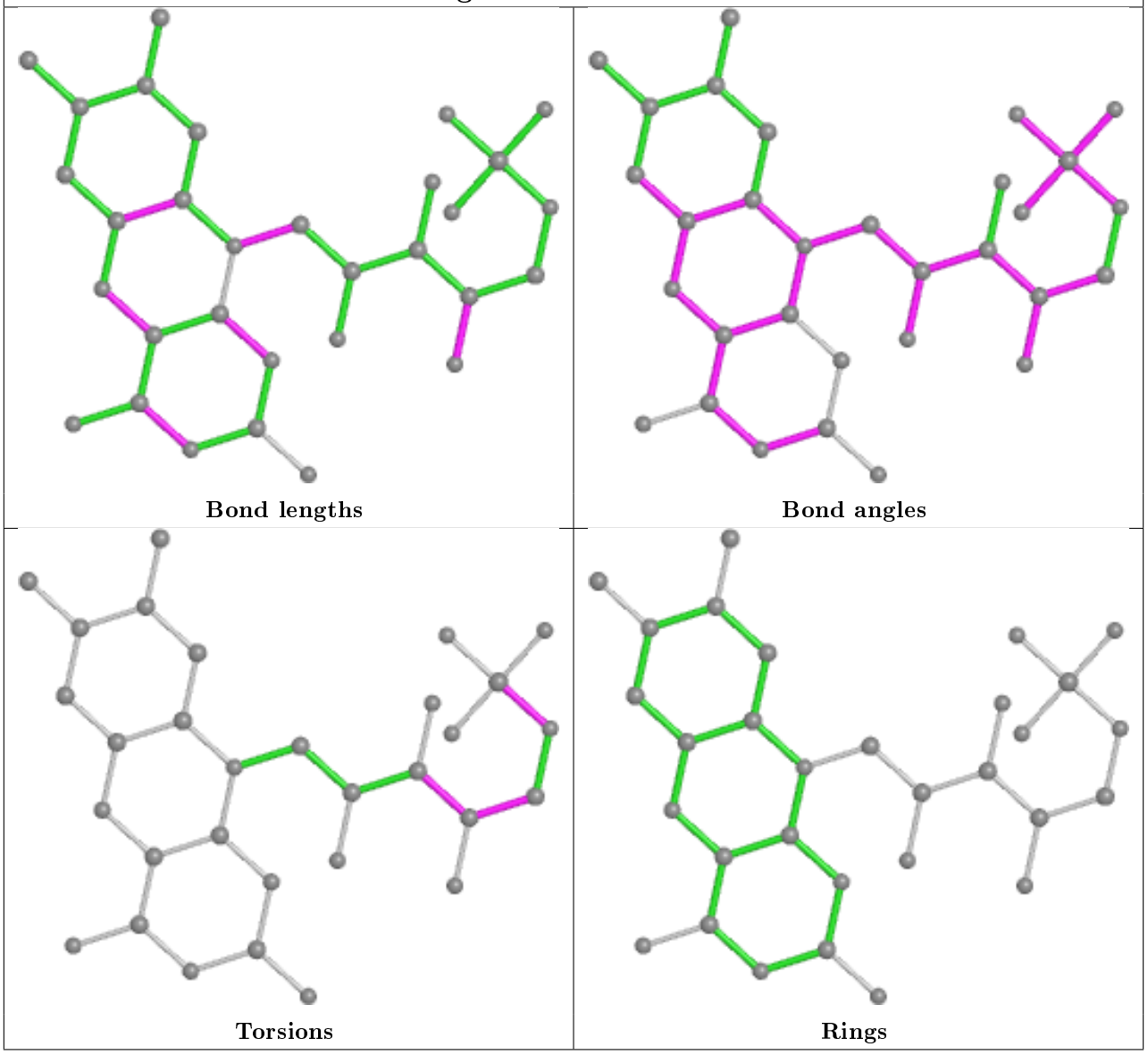


Torsions



Rings

Ligand FMN A 2474



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.