wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 06:53 PM EDT

PDB ID	:	1LM1
Title	:	Structural studies on the synchronization of catalytic centers in glutamate synthase: native enzyme
Authors	:	van Den Heuvel, R.H.; Ferrari, D.; Bossi, R.T.; Ravasio, S.; Curti, B.; Vanoni, M.A.; Florencio, F.J.; Mattevi, A.
Deposited on	:	2002-04-30
Resolution	:	2.80 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

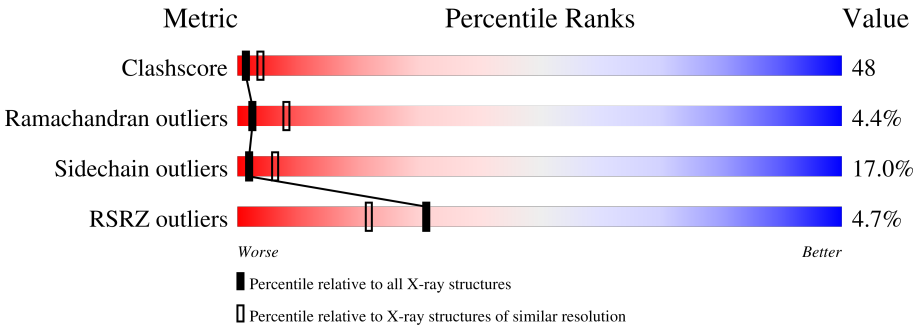
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	1520	5% 39% 44% 12%

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	ACT	A	2074	-	-	X	-
2	ACT	A	2075	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	F3S	A	2072	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11395 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.

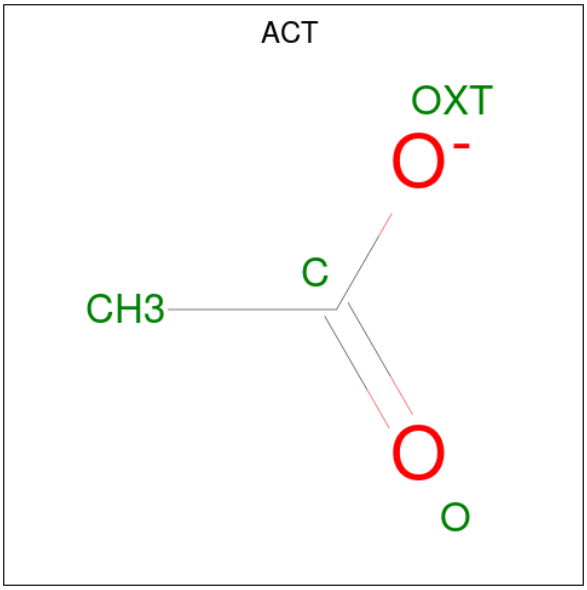
- Molecule 1 is a protein called Ferredoxin-dependent glutamate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1475	Total	C	N	O	S	0	0	0
			11311	7137	1970	2148	56			

There are 3 discrepancies between the modelled and reference sequences:

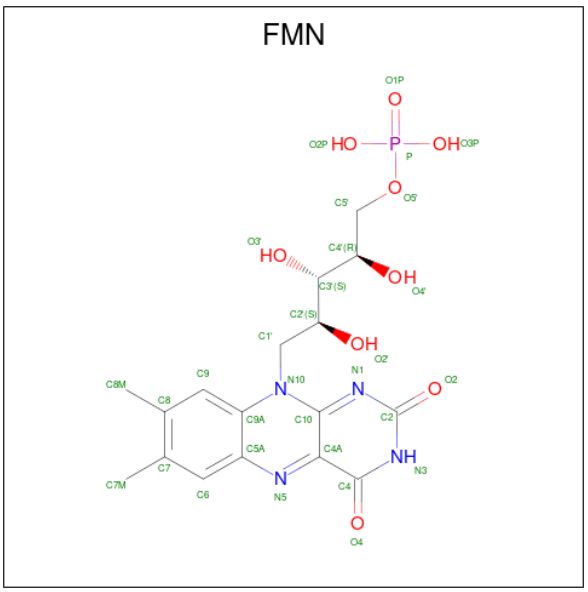
Chain	Residue	Modelled	Actual	Comment	Reference
A	578	ASP	THR	conflict	UNP P55038
A	581	THR	ASP	conflict	UNP P55038
A	1507	ASN	GLY	conflict	UNP P55038

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



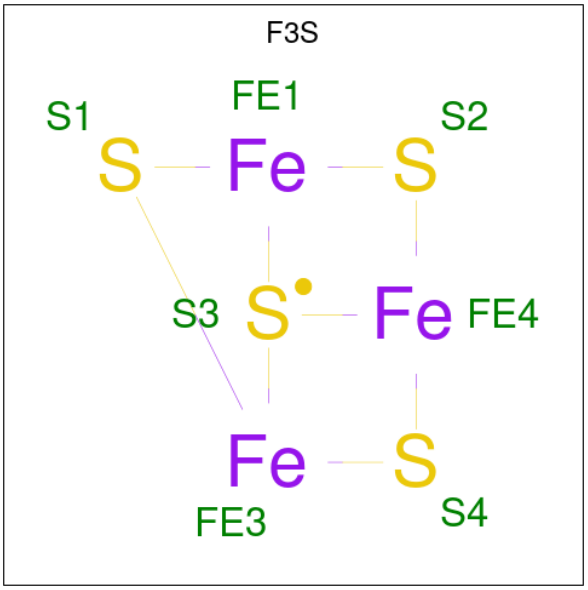
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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



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

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



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

- Molecule 5 is water.

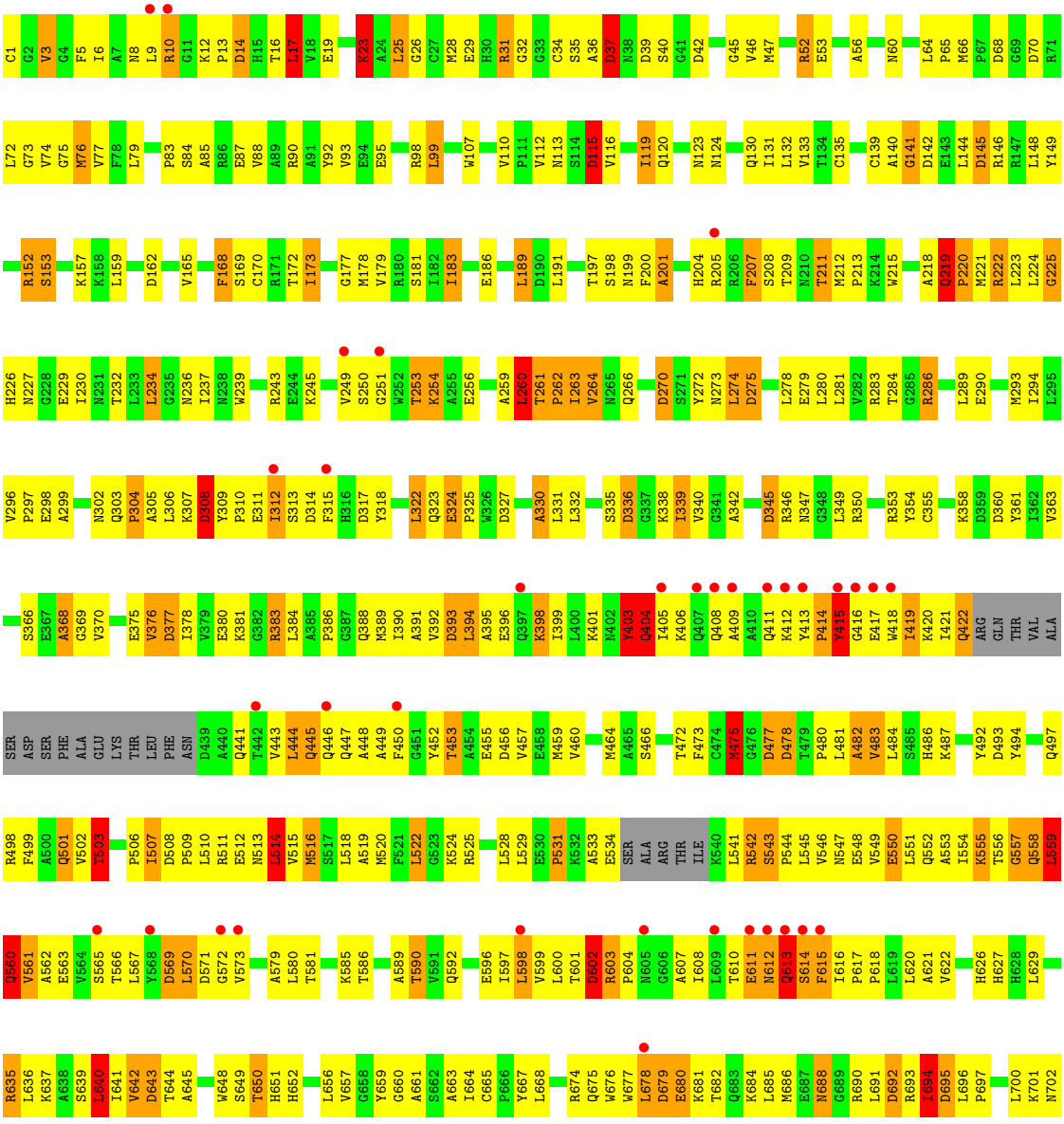
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		

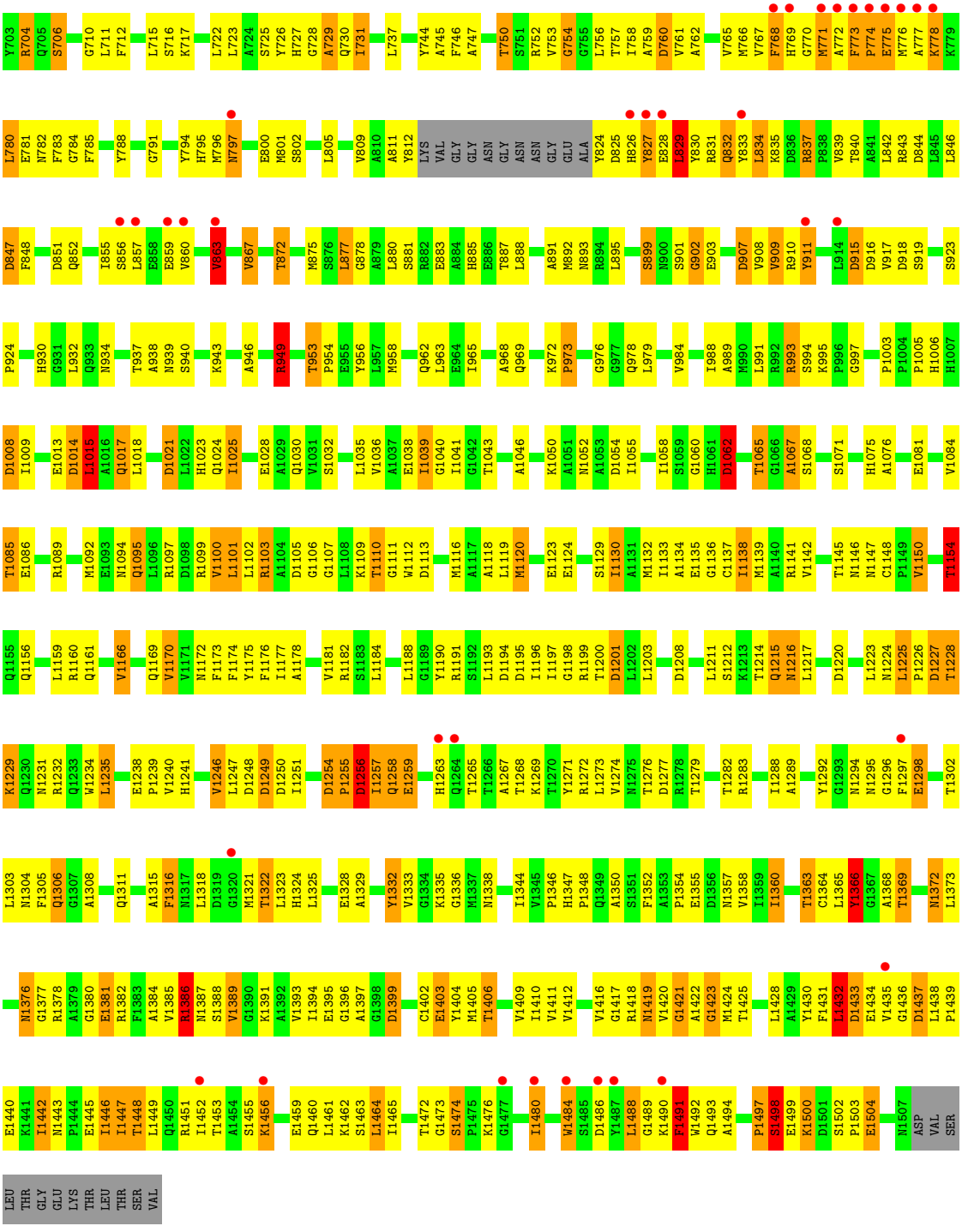
3 Residue-property plots (i)

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

• Molecule 1: Ferredoxin-dependent glutamate synthase

Chain A:




Y703 R704 Q705 S706 G710 L711 F712 L715 S716 K717 L722 L723 A724 S725 Y726 H727 G728 A729 Q730 I731 L737 Y744 A745 F746 A747 T750 S751 R752 V753 G754 G755 L756 T757 I758 A759 D760 V761 A762 V765 M766 V767 F768 H769 G770 M771 A772 F773 P774 E775 M776 A777 K778 K779
L780 E781 N782 F783 G784 F785 Y788 G791 Y794 H795 M796 N797 E800 M801 S802 L805 V809 A810 A811 Y812 LYS VAL GLY GLY ASN GLY ASN ASN GLY GLU ALA Y824 D825 H826 Y827 E828 L829 Y830 R831 Q832 Y833 L834 K835 D836 R837 P838 V839 T840 A841 L842 R843 D844 L845 L846
D847 F848 D851 Q852 I855 S856 L857 E858 E859 V860 V863 V867 T872 M875 S876 L877 G878 A879 L880 S881 H882 E883 A884 H885 E886 T887 L888 A891 M892 N893 R894 L895 S899 N900 S901 G902 E903 D907 V908 V909 R910 Y911 L914 D915 D916 V917 D918 S919 S923
P924 H930 G931 L932 Q933 N934 T937 A938 N939 S940 K943 A946 R949 T953 P954 E955 Y956 L957 M958 Q962 L963 E964 I965 A968 Q969 K972 P973 G976 G977 Q978 L979 V984 I988 A989 M990 L991 R992 R993 S994 K995 P996 G997 P1003 P1004 P1005 H1006 H1007
D1008 I1009 E1013 D1014 L1015 A1016 Q1017 L1018 D1021 L1022 H1023 Q1024 I1025 E1028 A1029 Q1030 V1031 S1032 L1035 V1036 A1037 E1038 I1039 G1040 I1041 G1042 T1043 A1046 K1050 A1051 N1052 A1053 D1054 I1055 I1058 S1059 G1060 H1061 D1062 T1065 G1066 A1067 S1068 S1071 H1075 A1076 E1081 V1084
T1085 E1086 R1089 M1092 E1093 N1094 Q1095 L1096 R1097 D1098 R1099 V1100 L1101 L1102 R1103 A1104 D1105 G1106 G1107 L1108 K1109 T1110 G1111 W1112 D1113 M1116 A1117 A1118 L1119 M1120 E1123 E1124 S1129 I1130 A1131 M1132 I1133 A1134 E1135 G1136 C1137 I1138 M1139 A1140 R1141 V1142 T1145 N1146 N1147 C1148 P1149 V1150 T1154
Q1155 Q1156 L1159 R1160 Q1161 V1166 Q1169 V1170 V1171 N1172 F1173 F1174 Y1175 F1176 I1177 A1178 V1181 R1182 S1183 L1184 L1188 G1189 Y1190 R1191 S1192 L1193 D1194 D1195 I1196 I1197 G1198 R1199 T1200 D1201 L1202 L1203 D1208 L1211 S1212 K1213 T1214 Q1215 N1216 L1217 D1220 L1223 N1224 L1225 P1226 D1227 T1228
K1229 Q1230 N1231 R1232 Q1233 W1234 L1235 E1238 P1239 V1240 H1241 V1246 L1247 D1248 D1249 D1250 I1251 D1254 P1255 D1256 I1257 Q1258 E1259 H1263 Q1264 T1265 T1266 A1267 T1268 K1269 T1270 Y1271 R1272 L1273 V1274 N1275 T1276 D1277 R1278 T1279 T1282 R1283 I1288 A1289 Y1292 G1293 N1294 N1295 G1296 F1297 E1298 T1302
L1303 N1304 F1305 Q1306 G1307 A1308 Q1311 A1315 F1316 N1317 L1318 D1319 G1320 M1321 T1322 L1323 H1324 L1325 E1328 A1329 Y1332 V1333 G1334 K1335 G1336 M1337 N1338 I1344 V1345 P1346 H1347 P1348 Q1349 A1350 S1351 F1352 A1353 P1354 E1355 D1356 N1357 V1358 I1359 I1360 T1363 C1364 L1365 Y1366 G1367 A1368 T1369 N1372 L1373
N1376 G1377 R1378 A1379 G1380 E1381 R1382 F1383 A1384 V1385 R1386 N1387 S1388 V1389 G1390 K1391 A1392 V1393 I1394 E1395 G1396 A1397 C1398 D1399 C1402 E1403 Y1404 M1405 T1406 V1409 I1410 V1411 V1412 V1416 G1417 R1418 N1419 V1420 G1421 A1422 G1423 M1424 T1425 L1428 A1429 Y1430 F1431 L1432 D1433 E1434 V1435 G1436 D1437 L1438 P1439
E1440 K1441 I1442 N1443 P1444 E1445 I1446 I1447 T1448 L1449 Q1450 R1451 I1452 T1453 A1454 S1455 K1456 E1459 Q1460 L1461 K1462 S1463 L1464 I1465 T1472 G1473 S1474 P1475 K1476 G1477 I1480 W1484 S1485 D1486 Y1487 L1488 G1489 K1490 F1491 W1492 Q1493 A1494 P1497 S1498 E1499 K1500 D1501 S1502 P1503 E1504 N1507 ASP VAL SER
LEU THR GLY GLU LYS THR LEU THR SER VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	166.08Å 166.08Å 219.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	129.10 – 2.80 61.52 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.7 (129.10-2.80) 99.4 (61.52-2.79)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.1.06	Depositor
R, R_{free}	0.236 , 0.287 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	72.0	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11395	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, F3S, ACT

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	0.95	13/11533 (0.1%)	1.18	88/15639 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1433	ASP	CB-CG	6.96	1.66	1.51
1	A	615	PHE	CE1-CZ	6.10	1.49	1.37
1	A	911	TYR	CD2-CE2	5.83	1.48	1.39
1	A	1008	ASP	CB-CG	-5.70	1.39	1.51
1	A	272	TYR	CE1-CZ	5.67	1.46	1.38

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	162	ASP	CB-CG-OD2	11.88	129.00	118.30
1	A	498	ARG	NE-CZ-NH1	-10.11	115.25	120.30
1	A	220	PRO	N-CD-CG	-8.50	90.45	103.20
1	A	1399	ASP	CB-CG-OD2	8.50	125.95	118.30
1	A	949	ARG	NE-CZ-NH2	-8.19	116.20	120.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ASN	Peptide
1	A	219	GLN	Peptide
1	A	403	TYR	Peptide
1	A	445	GLN	Peptide
1	A	99	LEU	Peptide

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	11311	0	11256	1070	0
2	A	8	0	6	6	0
3	A	31	0	19	4	0
4	A	7	0	0	3	0
5	A	38	0	0	7	0
All	All	11395	0	11281	1077	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 48.

The worst 5 of 1077 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:293:MET:SD	1:A:293:MET:CE	2.03	1.46
1:A:875:MET:SD	1:A:875:MET:CE	2.04	1.45
1:A:768:PHE:CE2	1:A:771:MET:HG2	1.55	1.42
1:A:686:MET:CE	1:A:692:ASP:HA	1.61	1.31
1:A:885:HIS:HD2	1:A:910:ARG:NH2	1.32	1.25

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	1467/1520 (96%)	1232 (84%)	171 (12%)	64 (4%)	2 8

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	395	ALA
1	A	403	TYR
1	A	414	PRO
1	A	415	TYR

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	1200/1236 (97%)	996 (83%)	204 (17%)	2 6

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	837	ARG
1	A	1100	VAL
1	A	1480	ILE
1	A	867	VAL
1	A	1013	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1372	ASN
1	A	1376	ASN

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Mol	Chain	Res	Type
1	A	1493	GLN
1	A	675	GLN
1	A	652	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	FMN	A	2070	-	33,33,33	1.18	2 (6%)	48,50,50	1.55	12 (25%)
2	ACT	A	2075	-	3,3,3	0.79	0	3,3,3	1.39	0
4	F3S	A	2072	1	0,9,9	-	-	-		
2	ACT	A	2074	-	3,3,3	0.77	0	3,3,3	1.92	2 (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	F3S	A	2072	1	-	-	0/3/3/3
3	FMN	A	2070	-	-	6/18/18/18	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2070	FMN	C4A-N5	2.97	1.36	1.30
3	A	2070	FMN	C4A-C10	-2.79	1.35	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2070	FMN	C8M-C8-C7	-3.67	113.21	120.74
3	A	2070	FMN	C4A-C10-N10	3.37	121.41	116.48
3	A	2070	FMN	C4-N3-C2	-3.02	120.06	125.64
3	A	2070	FMN	O4-C4-C4A	-2.69	119.46	126.60
2	A	2074	ACT	OXT-C-O	-2.56	112.61	122.05

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2070	FMN	C5'-O5'-P-O2P
3	A	2070	FMN	C5'-O5'-P-O3P
3	A	2070	FMN	C5'-O5'-P-O1P
3	A	2070	FMN	C4'-C5'-O5'-P
3	A	2070	FMN	O3'-C3'-C4'-O4'

There are no ring outliers.

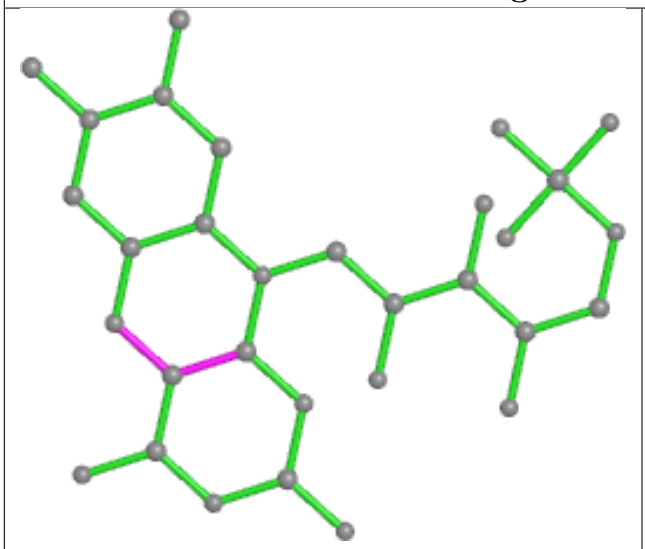
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2070	FMN	4	0
2	A	2075	ACT	5	0
4	A	2072	F3S	3	0
2	A	2074	ACT	6	0

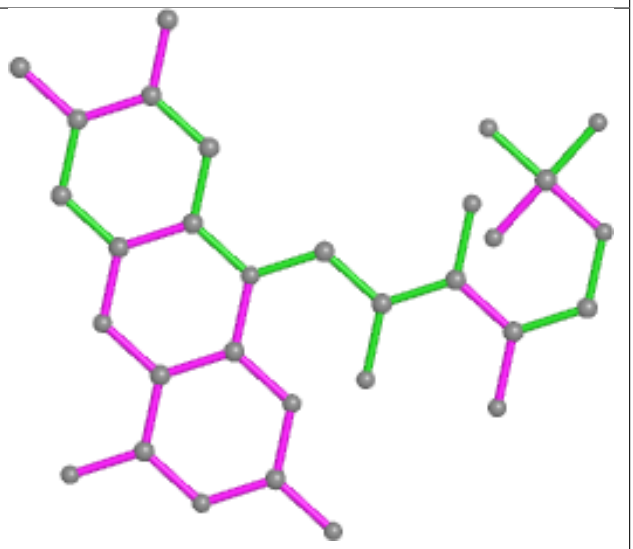
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

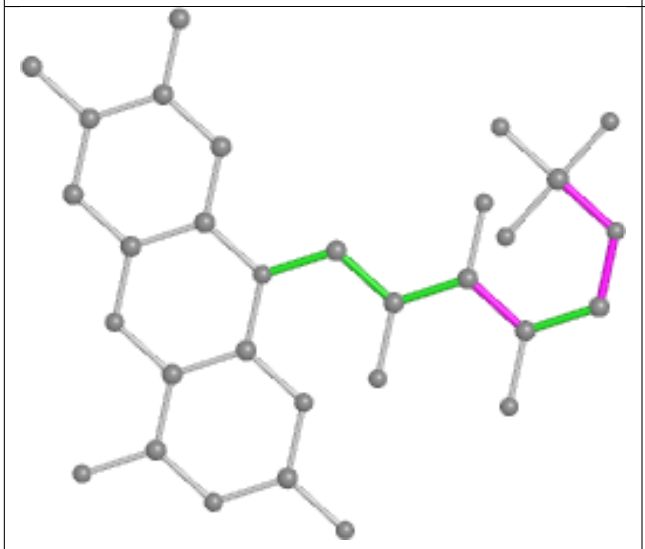
Ligand FMN A 2070



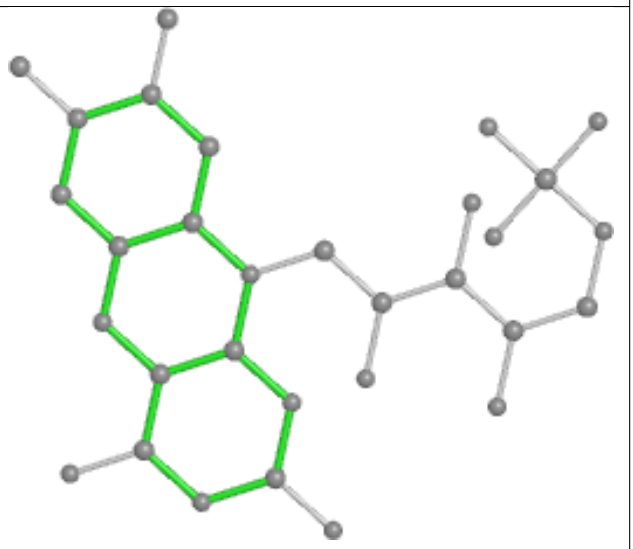
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} 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	1475/1520 (97%)	0.12	70 (4%)	31	22	24, 34, 41, 85	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	TYR	5.8
1	A	415	TYR	5.6
1	A	613	GLN	5.4
1	A	1487	TYR	5.0
1	A	411	GLN	4.8

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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
2	ACT	A	2074	4/4	0.84	0.39	61,62,63,63	0
2	ACT	A	2075	4/4	0.93	0.25	59,60,62,62	0

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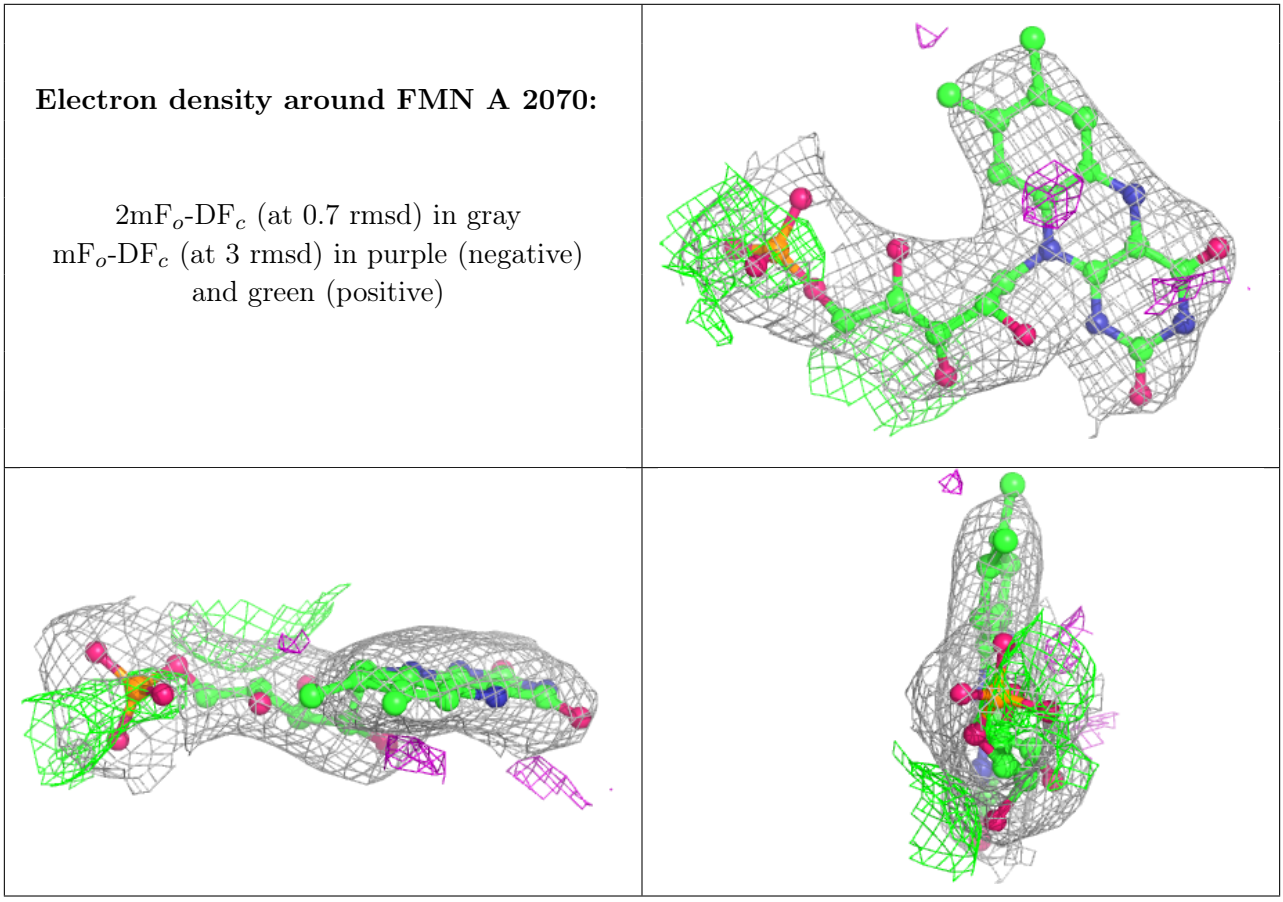
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FMN	A	2070	31/31	0.98	0.22	53,57,60,62	0
4	F3S	A	2072	7/7	1.00	0.15	60,63,68,70	0

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 FMN A 2070:

$2mF_o$-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.