wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 06:15 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

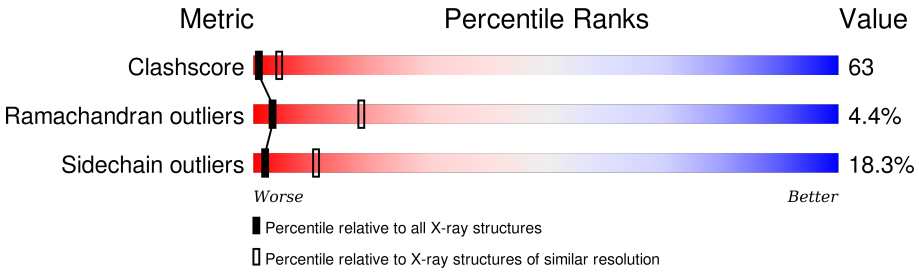
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (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. 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.

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
5	F3S	A	2476	-	-	X	-
5	F3S	B	2476	-	-	X	-

2 Entry composition

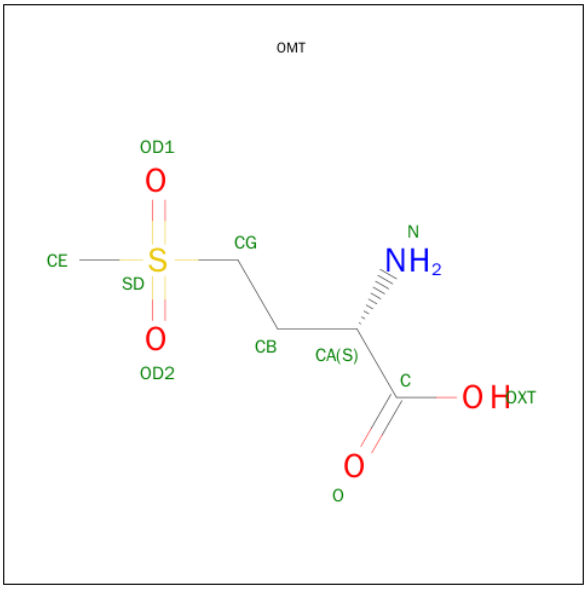
There are 5 unique types of molecules in this entry. The entry contains 22478 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

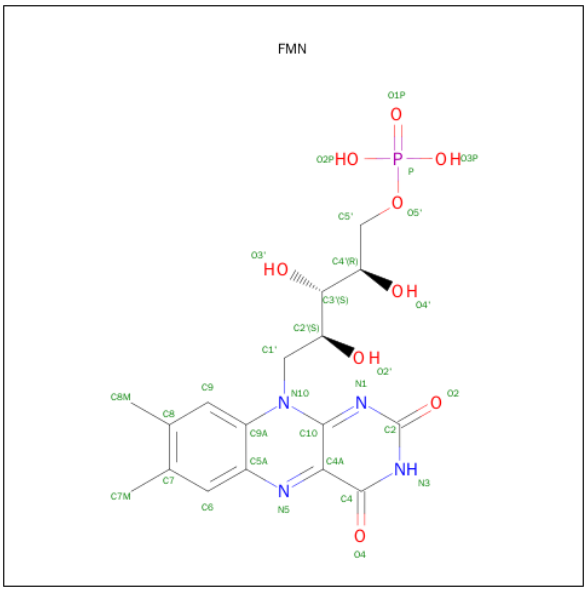
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1452	Total	C	N	O	S	0	0	0
			11180	7018	2005	2098	59			
1	B	1452	Total	C	N	O	S	0	0	0
			11180	7018	2005	2098	59			

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



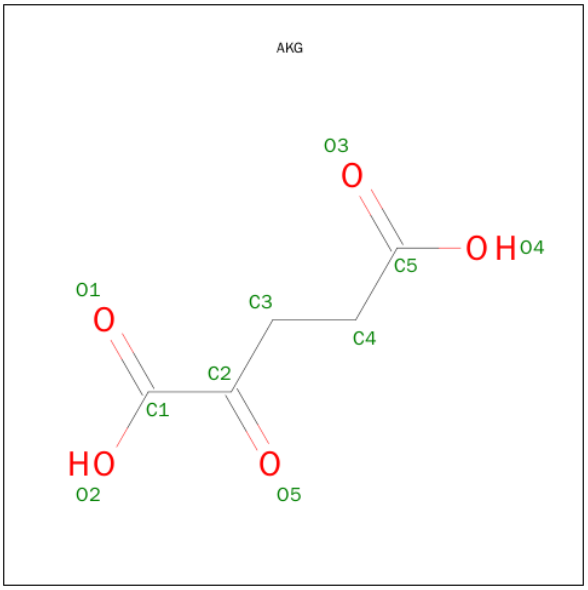
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			11	5	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			11	5	1	4	1		

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



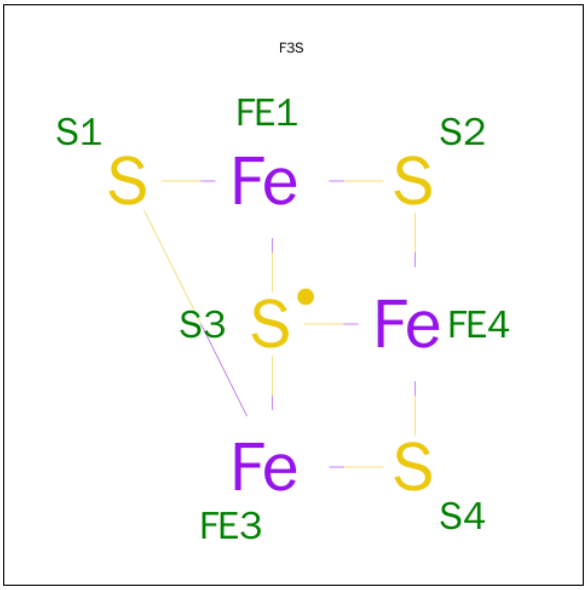
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- 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

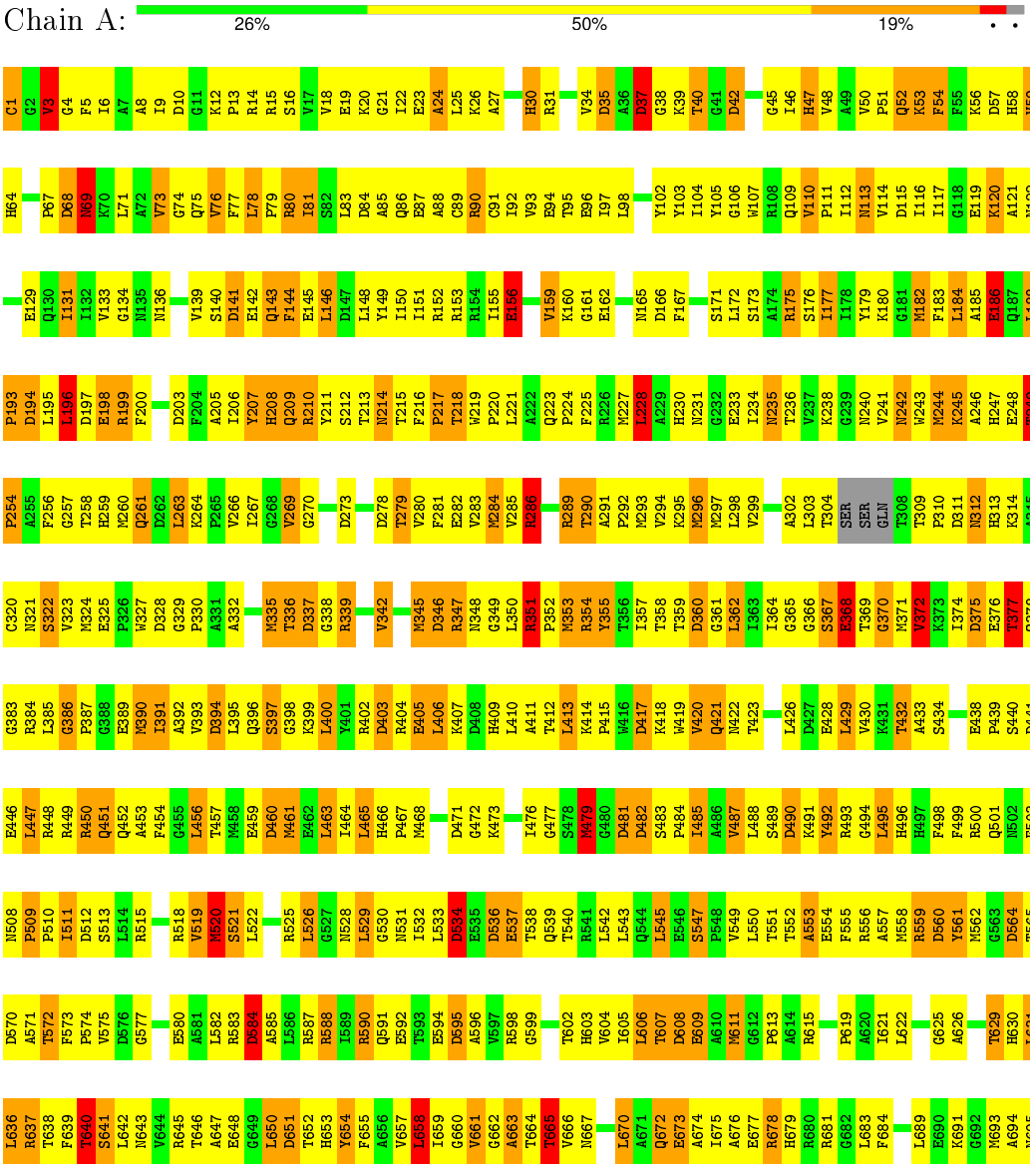
3 Residue-property plots (i)

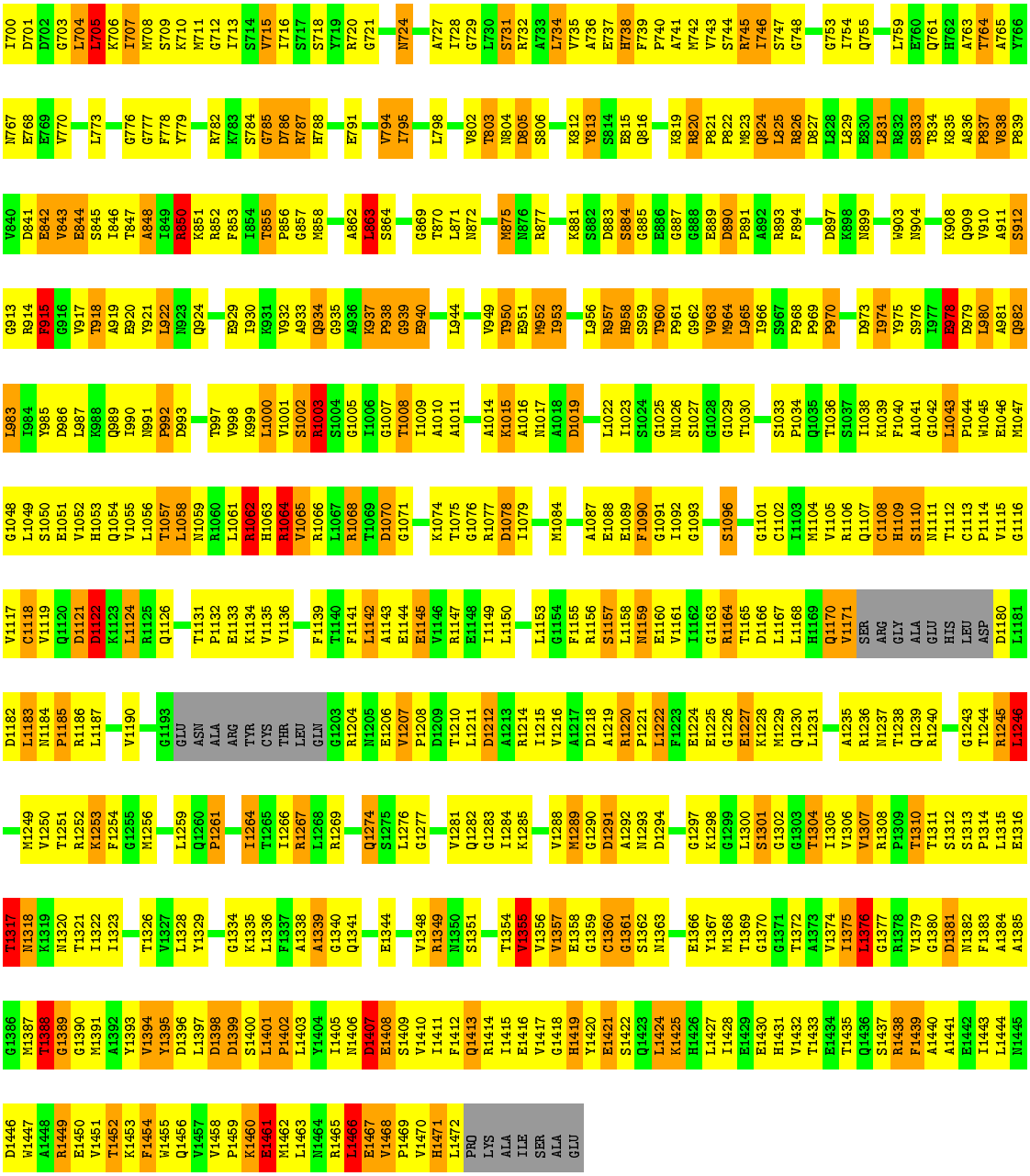
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN

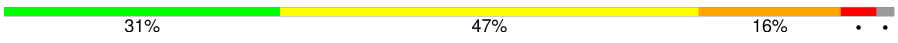
Chain A:

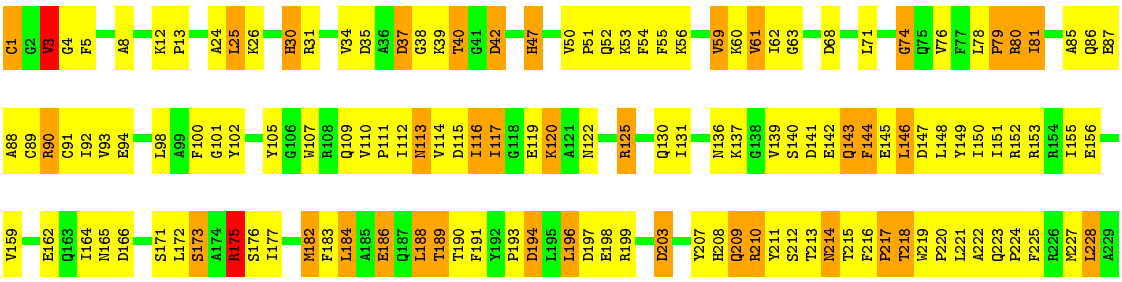




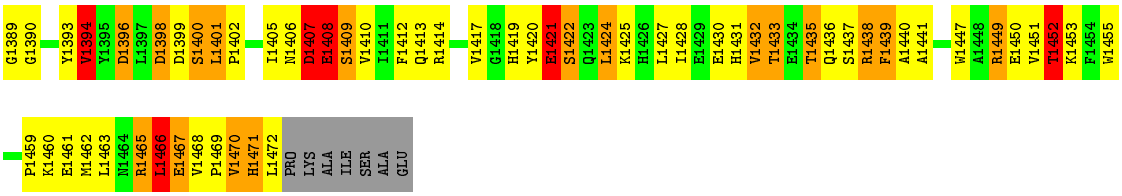
• Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN

Chain B:





H230 N231 G232 E233 I234 N235 T236 V237 K238 G239 N240 V241 N242 W243 M244 K245 E248 T249 R250 M251 E252 H253 P254 A255 F256 G257 T258 H259 M260 Q261 D262 L263 V266 I267 G268 V269 G270 S274 D278 T279 V280 F281 E282 V283 M284 V285 R286 R289 T290 A291 P292 M293 V294 K295 W296
M297 L298 V299 A302 L303 T304 SER SER GLN T308 T309 P310 D311 N312 H313 K314 A315 I316 I317 Q318 Y319 C320 N321 S322 V323 M324 E325 P326 W327 D328 G329 P330 D337 G338 R339 V342 G343 G344 M345 D346 R347 N348 G349 L350 R351 P352 M353 R354 Y355 T359 D360 G361 L362 I363 I364 G365
G366 S367 E368 T369 I374 D375 E376 T377 Q378 V379 I380 E381 L385 G386 P387 G388 E389 M390 V393 D394 L395 Q396 S397 G398 K399 R402 D403 R404 E405 L406 K407 D408 H409 L410 A411 T412 L413 K414 P415 W416 D417 K418 W419 V420 Q421 N422 T423 L426 D427 E428 L429 V430 G437 E438
P439 S440 D441 M442 D443 K444 A445 E446 L447 R448 R449 R450 Q451 Q452 A453 F454 G455 L456 T457 N458 E459 D460 M461 E462 L463 I464 L465 H466 P467 D471 G472 K473 E474 A475 I476 G477 S478 M479 G480 D481 D482 S483 P484 I485 A486 V487 L488 S489 D490 K491 Y492 R493 G494 L495 H496 H497 F498 P499 R500
Q501 N502 F503 S504 Q505 N508 P509 P510 I511 D512 S513 L514 R515 R518 V519 M520 S521 L522 R525 L526 G527 N528 L529 G530 N531 I532 L533 D534 E535 D536 E537 T538 Q539 T540 R541 L542 L543 Q544 L545 E546 S547 P548 V549 L550 T551 T552 A553 E554 F555 R556 A557 M558 R559 D560 Y561 M562 G563
D564 T565 E568 I569 D570 A571 T572 F573 P574 V575 D576 G577 E580 A581 L582 R583 D584 A585 L586 R587 R588 I589 R590 Q591 E592 T593 E594 D595 A596 V597 R598 T602 H603 V604 I605 L606 T607 D608 E609 A610 M611 G612 P613 A614 R615 A616 A617 I618 P619 A620 I621 L622 A623 T624 G625 A626 V627
H628 T629 H630 L631 I632 R633 S634 N635 L636 R637 T638 F639 T640 S641 L642 N643 V644 R645 T646 A647 E648 G649 L650 D651 T652 H653 Y654 F655 A656 V657 L658 I659 G660 V661 G662 A663 T664 T665 V666 N667 A668 Y669 L670 A671 Q672 E673 A674 I675 A676 E677 R678 H679 R680 R681 G682 L683 F684 M687 P688
L689 E690 K691 G692 M693 A694 N695 Y696 K697 K698 A699 I700 D701 D702 G703 L704 L705 K706 I707 K710 S714 S717 S718 Y719 R720 G721 G722 F725 E726 A727 I728 G729 L730 S731 R732 A733 L734 V735 H738 F739 P740 A741 M742 V743 S744 R745 I746 S747 G748 L751 N752 G753 I754 Q755
K756 K757 V758 L759 E760 Q761 H762 A763 T764 A765 Y766 M767 E768 E769 V770 L773 F774 V775 G776 G777 F778 Y779 R780 F781 R782 D786 R787 H788 G789 W790 E791 G792 G793 V794 I795 H796 T797 L798 A801 V802 T803 N804 D805 S806 Y807 T808 T809 F810 K811 K812 Y813 S814 E815 Q816 V817 N818 K819
R820 P821 P822 M823 Q824 L825 R826 D827 L828 L829 E830 L831 R832 S833 T834 K835 V838 P839 V840 D841 E842 V843 E844 S845 I846 T847 A848 I849 R850 K851 R852 F853 I854 T855 P856 G857 M858 S859 M860 G861 A862 L863 S864 P865 E866 A867 H868 G869 T870 L871 N872 V873 A874 M875 N876 R877 I878 G879 A880
D883 S884 G885 E886 G887 G888 E889 D890 P891 F894 D897 K898 N899 I907 K908 Q909 V910 A911 S912 G913 R914 F915 G916 V917 T918 A919 E920 Y921 L922 E927 L928 E929 I930 K931 V932 A933 Q934 K937 P938 G939 E940 G941 G942 Q943 L944 P945 G946 F947 K948 T950 E951 M952 I953
A954 R955 L956 R957 H958 S959 T960 V963 M964 L965 I966 S967 P968 P969 P970 D973 I974 Y975 S976 I977 E978 D979 L980 A981 Q982 L983 I984 Y985 D986 L987 K988 Q989 I990 N991 P992 D993 T997 V998 K999 L1000 V1001 S1002 R1003 S1004 G1005 I1006 G1007 T1008 I1009 A1010 A1011 G1012 V1013 A1014 K1015 A1016 N1017
A1018 L1022 N1026 T1030 G1031 A1032 S1033 P1034 I1038 K1039 F1040 A1041 G1042 L1043 P1044 W1045 E1046 M1047 G1048 L1049 S1050 E1051 V1052 H1053 Q1054 V1055 L1056 T1057 L1058 N1059 R1060 L1061 R1062 H1063 R1064 V1065 R1066 L1067 R1068 T1069 D1070 G1071 K1074 T1075 G1076 R1077 D1078 I1079 V1080 I1081 M1084 E1088 E1089
F1090 G1091 I1092 G1093 T1094 A1095 S1096 L1097 C1102 I1103 M1104 V1105 R1106 Q1107 C1108 H1109 S1110 N1111 T1112 C1113 P1114 V1115 V1119 Q1120 D1121 D1122 K1123 L1124 R1125 Q1126 K1127 F1128 V1129 G1130 T1131 P1132 E1133 K1134 V1135 V1136 N1137 L1138 F1139 T1140 F1141 L1142 A1143 E1144 E1145 V1146 R1147 A1151 G1152 L1153 G1154 F1155 R1156
S1157 L1158 M1159 E1160 V1161 I1162 G1163 R1164 T1165 D1166 L1167 L1168 H1169 Q1170 V1171 SER ARG GLY ALA GLU HIS LEU ASP D1180 L1181 D1182 L1183 N1184 P1185 R1186 L1187 V1190 D1191 P1192 G1193 GLU ASN ALA ARG TYR CYS THR LEU GLN G1203 R1204 N1205 E1206 V1207 P1208 D1209 T1210 L1211 D1212 I1215 V1216 A1217 D1218
A1219 R1220 P1221 L1222 M1229 Q1230 Y1233 R1236 M1237 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 M1325 T1326 V1327 L1328 Y1329 K1335 L1336 F1337 A1338 A1339 G1340 E1344 R1345 F1346 A1347 Y1348 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 will therefore be 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

Continued on next page...

Continued from previous page...

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%)	3 18
1	B	1444/1479 (98%)	1170 (81%)	211 (15%)	63 (4%)	3 18
All	All	2888/2958 (98%)	2322 (80%)	438 (15%)	128 (4%)	3 18

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%)	2 11
1	B	1184/1206 (98%)	965 (82%)	219 (18%)	2 10
All	All	2368/2412 (98%)	1935 (82%)	433 (18%)	2 11

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	$\#\|Z\| > 2$
2	OMT	A	2473	-	7,10,10	4.40	4 (57%)	8,14,14	4.87	6 (75%)
3	FMN	A	2474	-	32,33,33	1.37	5 (15%)	34,50,50	3.29	17 (50%)
4	AKG	A	2475	-	3,9,9	4.56	2 (66%)	4,11,11	2.81	2 (50%)
5	F3S	A	2476	1	0,9,9	0.00	-	0,15,15	0.00	-
2	OMT	B	2473	-	7,10,10	4.33	4 (57%)	8,14,14	7.20	5 (62%)
3	FMN	B	2474	-	32,33,33	1.22	4 (12%)	34,50,50	2.70	15 (44%)
4	AKG	B	2475	-	3,9,9	4.91	2 (66%)	4,11,11	3.32	2 (50%)
5	F3S	B	2476	1	0,9,9	0.00	-	0,15,15	0.00	-

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
2	OMT	A	2473	-	-	0/6/10/10	0/0/0/0
3	FMN	A	2474	-	-	0/18/18/18	0/3/3/3
4	AKG	A	2475	-	-	0/3/9/9	0/0/0/0
5	F3S	A	2476	1	-	0/0/24/24	0/0/3/3
2	OMT	B	2473	-	-	0/6/10/10	0/0/0/0
3	FMN	B	2474	-	-	0/18/18/18	0/3/3/3
4	AKG	B	2475	-	-	0/3/9/9	0/0/0/0
5	F3S	B	2476	1	-	0/0/24/24	0/0/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2473	OMT	CG-SD	-7.15	1.69	1.78
2	A	2473	OMT	CG-SD	-6.95	1.69	1.78
2	A	2473	OMT	CB-CG	-6.87	1.45	1.52
2	B	2473	OMT	CB-CG	-5.90	1.46	1.52
3	A	2474	FMN	C9A-C5A	-2.80	1.36	1.42

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2473	OMT	OD2-SD-CG	-18.14	96.65	108.26
2	A	2473	OMT	OD2-SD-CE	-10.74	97.19	108.91
3	A	2474	FMN	O5'-P-O1P	-9.02	84.41	107.08
3	A	2474	FMN	O4'-C4'-C5'	-6.51	95.89	110.09
3	B	2474	FMN	O4'-C4'-C3'	-6.05	93.39	108.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 20 short contacts:

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

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.