wwPDB X-ray Structure Validation Summary Report (i)

Feb 11, 2024 – 04:28 PM EST

PDB ID	:	3G60
Title	:	Structure of P-glycoprotein Reveals a Molecular Basis for Poly-Specific Drug Binding
Authors	:	Aller, S.G.; Yu, J.; Ward, A.; Weng, Y.; Chittaboina, S.; Zhuo, R.; Harrell, P.M.; Trinh, Y.T.; Zhang, Q.; Urbatsch, I.L.; Chang, G.
Deposited on	:	2009-02-05
Resolution	:	4.40 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 (1)) were used in the production of this report:

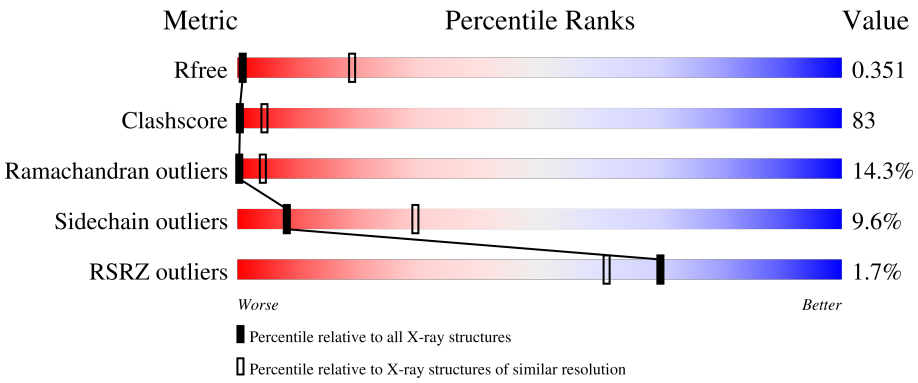
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 4.40 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	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)
RSRZ outliers	127900	1095 (5.08-3.70)

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	1284	2% 16% 59% 15% • 8%
1	B	1284	2% 16% 59% 16% • 8%

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	0JZ	A	6001	-	-	-	X
2	0JZ	B	6002	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18414 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.

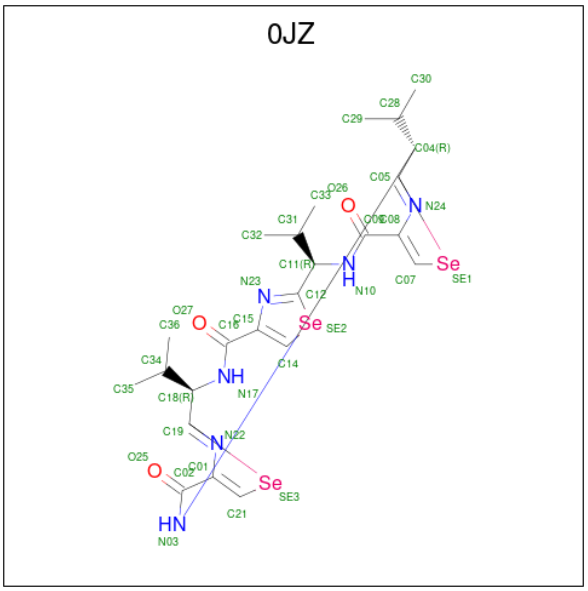
- Molecule 1 is a protein called Multidrug resistance protein 1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1182	9171	5895	1552	1686	38	0	0	0
1	B	1182	9171	5895	1552	1686	38	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1277	TYR	-	expression tag	UNP Q5I1Y5
A	1278	VAL	-	expression tag	UNP Q5I1Y5
A	1279	HIS	-	expression tag	UNP Q5I1Y5
A	1280	HIS	-	expression tag	UNP Q5I1Y5
A	1281	HIS	-	expression tag	UNP Q5I1Y5
A	1282	HIS	-	expression tag	UNP Q5I1Y5
A	1283	HIS	-	expression tag	UNP Q5I1Y5
A	1284	HIS	-	expression tag	UNP Q5I1Y5
B	1277	TYR	-	expression tag	UNP Q5I1Y5
B	1278	VAL	-	expression tag	UNP Q5I1Y5
B	1279	HIS	-	expression tag	UNP Q5I1Y5
B	1280	HIS	-	expression tag	UNP Q5I1Y5
B	1281	HIS	-	expression tag	UNP Q5I1Y5
B	1282	HIS	-	expression tag	UNP Q5I1Y5
B	1283	HIS	-	expression tag	UNP Q5I1Y5
B	1284	HIS	-	expression tag	UNP Q5I1Y5

- Molecule 2 is (4R,11R,18R)-4,11,18-tri(propan-2-yl)-6,13,20-triselena-3,10,17,22,23,24-hexaa zatetracyclo[17.2.1.1 5,8 .1 12,15]tetracosa-1(21),5(24),7,12(23),14,19(22)-hexaene-2,9,16-tri one (three-letter code: 0JZ) (formula: $C_{24}H_{30}N_6O_3Se_3$).



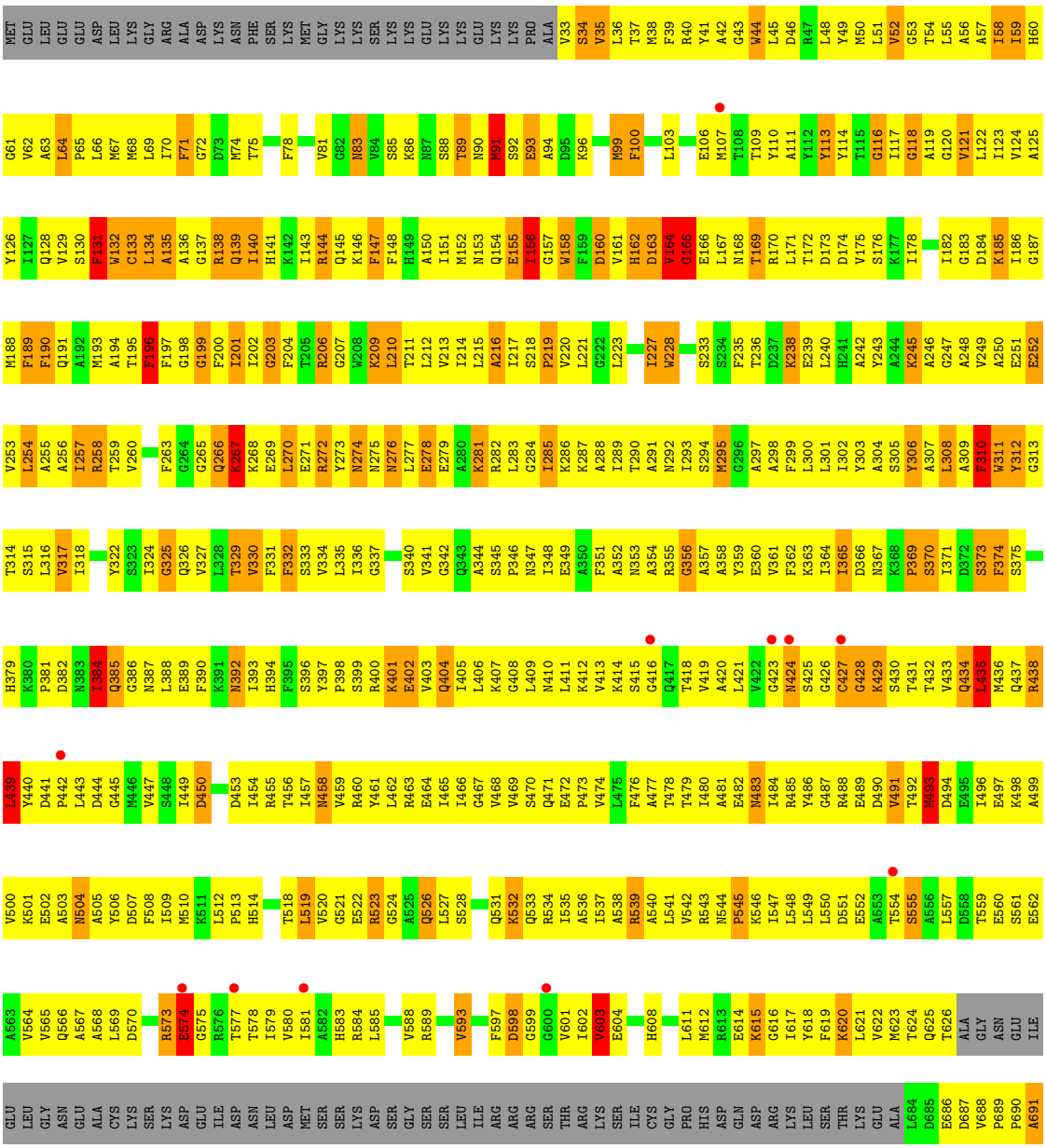
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	Se		
2	A	1	36	24	6	3	3	0	0
			Total	C	N	O	Se		
2	B	1	36	24	6	3	3	0	0

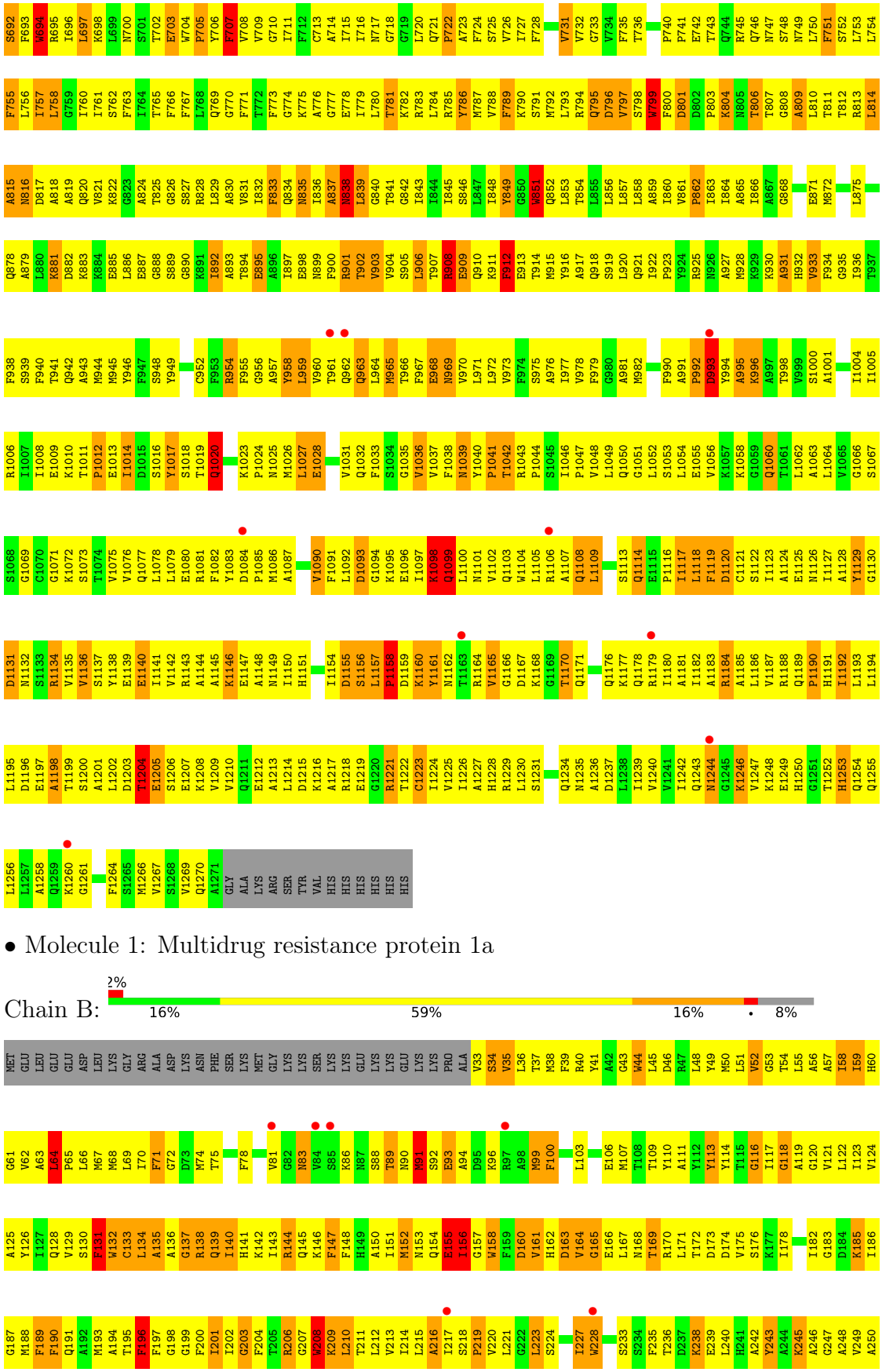
3 Residue-property plots (i)

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: Multidrug resistance protein 1a

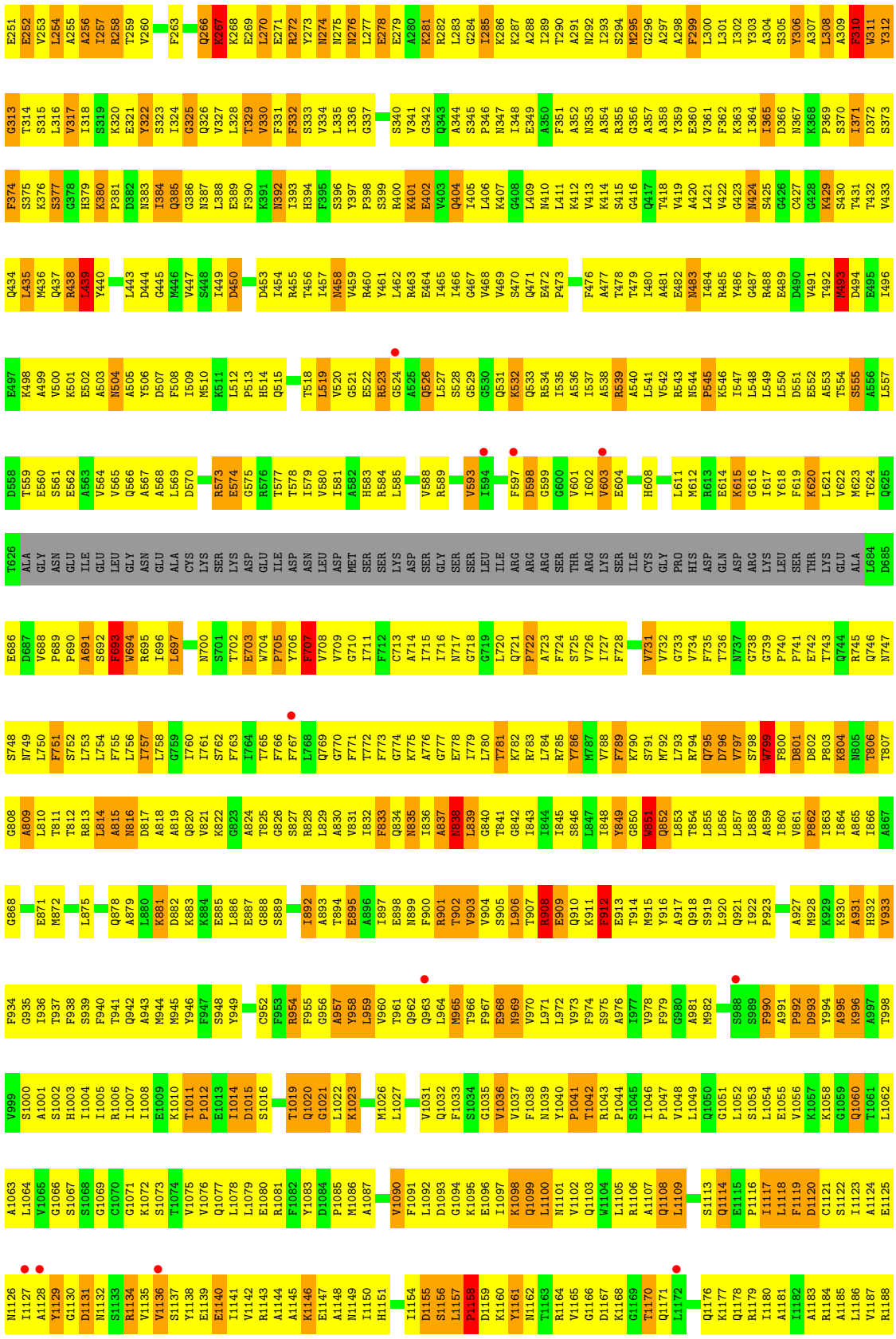
Chain A: 2% 16% 59% 15% 8%

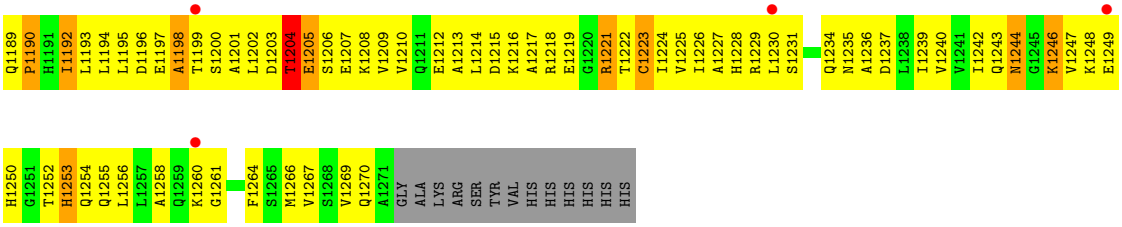




• Molecule 1: Multidrug resistance protein 1a

Chain B: 2% 16% 59% 16% • 8%


N1126 I1127 A1128 Y1129 G1130 D1131 N1132 S1133 R1134 V1135 V1136 S1137 Y1138 E1139 E1140 I1141 V1142 R1143 A1144 A1145 K1146 E1147 A1148 N1149 I1150 H1151
A1063 L1064 V1065 G1066 S1067 S1068 G1069 C1070 G1071 K1072 S1073 T1074 V1075 V1076 Q1077 L1078 L1079 E1080 R1081 F1082 Y1083 D1084 P1085 M1086 A1087
V999 S1000 A1001 S1002 H1003 I1004 I1005 R1006 I1007 I1008 E1009 K1010 T1011 P1012 E1013 I1014 D1015 S1016 T1019 Q1020 G1021 L1022 A957 Y958 L959 V960 V961 Q962 Q963 L964 M965 T966 F967 E968 N969 V970 V1037 F1038 N1039 Y1040 P1041 T1042 R1043 P1044 S1045 I1046 P1047 V1048 L1049 Q1050 G1051 L1052 S1053 L1054 E1055 V1056 K1057 K1058 G1059 Q1060 T1061 L1062
F934 G935 I936 T937 F938 S939 F940 T941 Q942 A943 M944 M945 Y946 F947 S948 Y949 C952 F953 R954 F955 G956 A957 Y958 L959 V960 V961 Q962 Q963 L964 M965 T966 F967 E968 N969 V970 V1037 F1038 N1039 Y1040 P1041 T1042 R1043 P1044 S1045 I1046 P1047 V1048 L1049 Q1050 G1051 L1052 S1053 L1054 E1055 V1056 K1057 K1058 G1059 Q1060 T1061 L1062
G868 E871 M872 L875 Q878 A879 L880 K881 D882 K883 K884 E885 L886 E887 G888 S889 I892 A893 T894 A895 E896 I897 E898 N899 F900 R901 T902 V903 V904 S905 L906 T907 R908 E909 Q910 K911 F912 E913 T914 M915 Y916 A917 Q918 S919 L920 Q921 I922 P923 A927 M928 K929 K930 A931 H932 V933
G808 A809 L810 T811 T812 R813 L814 A815 N816 D817 A818 A819 Q820 V821 K822 G823 A824 T825 G826 S827 R828 L829 A830 V831 I832 F833 Q834 N835 I836 A837 N838 L839 G840 T841 G842 I843 I844 I845 S846 L847 I848 Y849 G850 W851 Q852 L853 T854 L855 L856 L857 L858 A859 I860 V861 P862 D862 I863 I864 A865 I866 A867
S748 N749 L750 F751 S752 L753 L754 F755 L756 I757 L758 G759 I760 I761 S762 F763 I764 T765 F766 F767 L768 Q769 G770 F771 T772 F773 G774 K775 A776 G777 E778 I779 L780 T781 K782 R783 L784 K785 Y786 M787 V788 F789 K790 S791 M792 L793 R794 Q795 D796 V797 S798 W799 F800 D801 D802 P803 K804 N805 T806 T807
E686 D687 V688 P689 P690 A691 S692 F693 W694 R695 I696 L697 N700 S701 T702 E703 W704 P705 Y706 F707 V708 V709 G710 I711 F712 C713 A714 I715 I716 N717 G718 G719 L720 Q721 P722 A723 F724 S725 V726 I727 F728 V731 V732 G733 V734 F735 T736 N737 G738 G739 P740 P741 E742 T743 Q744 R745 Q746 N747
T626 ALA GLY ASN GLU ILE GLU LEU GLY ASN GLU ALA CYS LYS SER LYS ASP GLU ILE ASP ASN LEU ASP MET SER SER LYS ASP SER GLY SER SER LEU ILE ARG ARG ARG SER THR ARG LYS SER ILE CYS GLY PRO HIS ASP GLN ASP ARG LYS LEU SER THR LYS GLU ALA L684 D685
D558 T559 E560 S561 E562 A563 V564 V565 Q566 A567 A568 L569 D570 R573 E574 G575 R576 T577 T578 I579 V580 I581 A582 H583 R584 L585 V588 R589 V593 T594 F597 D598 G599 G600 V601 I602 V603 E604 H608 L611 M612 R613 E614 K615 G616 I617 Y618 F619 K620 L621 V622 M623 T624 Q625
D558 T559 E560 S561 E562 A563 V564 V565 Q566 A567 A568 L569 D570 R573 E574 G575 R576 T577 T578 I579 V580 I581 A582 H583 R584 L585 V588 R589 V593 T594 F597 D598 G599 G600 V601 I602 V603 E604 H608 L611 M612 R613 E614 K615 G616 I617 Y618 F619 K620 L621 V622 M623 T624 Q625
E497 K498 A499 V500 K501 E502 A503 N504 A505 Y506 D507 F508 I509 M510 K511 L512 P513 H514 Q515 T518 L519 V520 G521 L522 R523 G524 A525 Q526 L527 S528 G529 G530 Q531 K532 Q533 R534 I535 A536 I537 A538 R539 A540 L541 V542 R543 N544 P545 K546 I547 L548 L549 L550 D551 E552 A553 T554 S555 A556 L557
Q434 L435 M436 Q437 R438 L439 Y440 L443 D444 G445 M446 V447 S448 I449 D450 D453 I454 R455 T456 I457 M458 V459 R460 Y461 L462 R463 Q464 I465 I466 G467 V468 V469 S470 Q471 E472 P473 F476 A477 T478 T479 I480 A481 E482 N483 I484 R485 Y486 G487 R488 E489 D490 V491 T492 M493 D494 E495 I496
F374 S375 K376 S377 G378 H379 K380 P381 D382 N383 I384 Q385 G386 N387 L388 E389 F390 K391 N392 I393 H394 F395 S396 Y397 P398 S399 R400 K401 E402 V403 Q404 I405 L406 K407 G408 L409 N410 L411 K412 V413 K414 S415 G416 Q417 T418 V419 A420 L421 V422 G423 N424 S425 G426 C427 G428 K429 S430 T431 T432 V433
G313 T314 S315 L316 V317 I318 S319 K320 E321 Y322 S323 I324 G325 Q326 V327 L328 T329 V330 F331 F332 S333 V334 L335 I336 G337 S340 V341 G342 Q343 A344 S345 P346 F350 F351 A352 N353 A354 R355 G356 A357 A358 Y359 E360 V361 F362 K363 I364 I365 D366 N367 K368 P369 S370 I371 D372 S373
E251 E252 V253 L254 A255 A256 I257 R258 T259 V260 F263 Q266 K267 K268 E269 L270 E271 R272 Y273 N274 N275 N276 L277 E278 E279 A280 K281 R282 L283 G284 I285 K286 K287 A288 I289 T290 A291 N292 I293 S294 M295 G296 A297 A298 F299 L300 L301 I302 Y303 A304 S305 Y306 A307 L308 A309 F310 W311 Y312


Q1189
P1190
H1191
I1192
L1193
L1194
L1195
D1196
E1197
A1198
T1199
S1200
A1201
L1202
D1203
T1204
E1205
S1206
E1207
K1208
V1209
V1210
Q1211
E1212
A1213
L1214
D1215
K1216
A1217
R1218
E1219
G1220
R1221
T1222
C1223
I1224
V1225
I1226
A1227
H1228
R1229
L1230
S1231
Q1234
N1235
A1236
D1237
L1238
I1239
V1240
V1241
I1242
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N1244
G1245
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V1247
K1248
E1249
H1250
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T1252
H1253
Q1254
Q1255
L1256
L1257
A1258
Q1259
K1260
G1261
F1264
S1265
M1266
V1267
S1268
V1269
Q1270
A1271
GLY
ALA
LYS
ARG
SER
TYR
VAL
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.63Å 115.09Å 374.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 4.40 49.02 – 4.31	Depositor EDS
% Data completeness (in resolution range)	94.7 (19.99-4.40) 93.3 (49.02-4.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	5.10 (at 4.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.314 , 0.365 0.297 , 0.351	Depositor DCC
R_{free} test set	2835 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å^2)	201.9	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 103.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	18414	wwPDB-VP
Average B, all atoms (Å^2)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 0JZ

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	0.41	1/9339 (0.0%)	0.70	13/12626 (0.1%)
1	B	0.41	0/9339	0.68	8/12626 (0.1%)
All	All	0.41	1/18678 (0.0%)	0.69	21/25252 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	851	TRP	CB-CG	5.17	1.59	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	427	CYS	N-CA-C	9.35	136.24	111.00
1	A	1098	LYS	N-CA-C	-7.80	89.94	111.00
1	A	164	VAL	N-CA-C	-7.79	89.98	111.00
1	A	267	LYS	N-CA-C	7.23	130.52	111.00
1	A	165	GLY	N-CA-C	-7.16	95.21	113.10

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	9171	0	9344	1558	0
1	B	9171	0	9344	1534	0
2	A	36	0	27	12	0
2	B	36	0	27	10	0
All	All	18414	0	18742	3089	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 83.

The worst 5 of 3089 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:797:VAL:O	1:B:801:ASP:HB2	1.45	1.15
1:A:523:ARG:HD3	1:A:524:GLY:H	0.99	1.13
1:B:523:ARG:HD3	1:B:524:GLY:H	0.98	1.12
1:B:858:LEU:O	1:B:862:PRO:HD2	1.51	1.11
1:B:1204:THR:O	1:B:1206:SER:N	1.83	1.10

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	1178/1284 (92%)	704 (60%)	302 (26%)	172 (15%)	0 4
1	B	1178/1284 (92%)	707 (60%)	305 (26%)	166 (14%)	0 4
All	All	2356/2568 (92%)	1411 (60%)	607 (26%)	338 (14%)	0 4

5 of 338 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	35	VAL
1	A	52	VAL
1	A	89	THR
1	A	133	CYS

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	976/1065 (92%)	884 (91%)	92 (9%)	8 30
1	B	976/1065 (92%)	880 (90%)	96 (10%)	8 29
All	All	1952/2130 (92%)	1764 (90%)	188 (10%)	8 29

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	238	LYS
1	B	694	TRP
1	B	254	LEU
1	B	332	PHE
1	B	771	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	437	GLN
1	B	963	GLN
1	B	515	GLN
1	B	805	ASN
1	B	1099	GLN

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)

2 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	0JZ	B	6002	-	21,39,39	1.74	4 (19%)	24,57,57	1.91	7 (29%)
2	0JZ	A	6001	-	21,39,39	2.04	5 (23%)	24,57,57	2.49	9 (37%)

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	0JZ	B	6002	-	-	4/24/48/48	0/3/4/4
2	0JZ	A	6001	-	-	4/24/48/48	0/3/4/4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6001	0JZ	C16-N17	5.48	1.46	1.34
2	B	6002	0JZ	C09-N10	4.44	1.43	1.34
2	A	6001	0JZ	C02-N03	4.39	1.43	1.34
2	A	6001	0JZ	C09-N10	3.88	1.42	1.34
2	B	6002	0JZ	C02-N03	3.70	1.42	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	6001	0JZ	C04-N03-C02	5.49	131.07	122.28
2	A	6001	0JZ	C18-N17-C16	5.23	130.66	122.28
2	A	6001	0JZ	C35-C34-C18	4.30	115.38	111.24
2	B	6002	0JZ	C33-C31-C11	3.77	114.87	111.24
2	B	6002	0JZ	C29-C28-C04	3.75	114.85	111.24

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	6001	0JZ	C05-C04-N03-C02
2	A	6001	0JZ	C28-C04-N03-C02
2	A	6001	0JZ	C19-C18-N17-C16
2	A	6001	0JZ	C34-C18-N17-C16
2	B	6002	0JZ	C05-C04-N03-C02

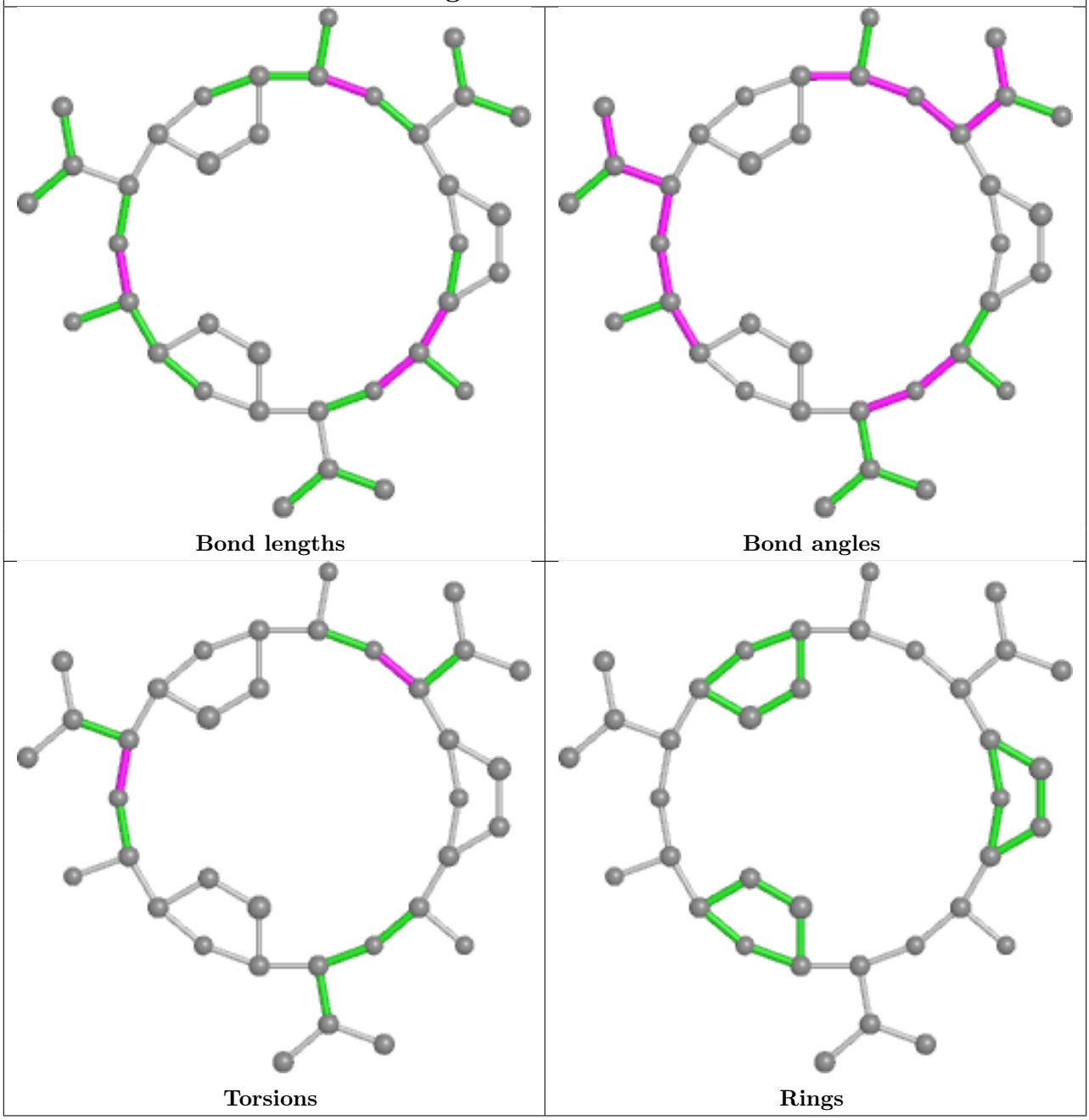
There are no ring outliers.

2 monomers are involved in 22 short contacts:

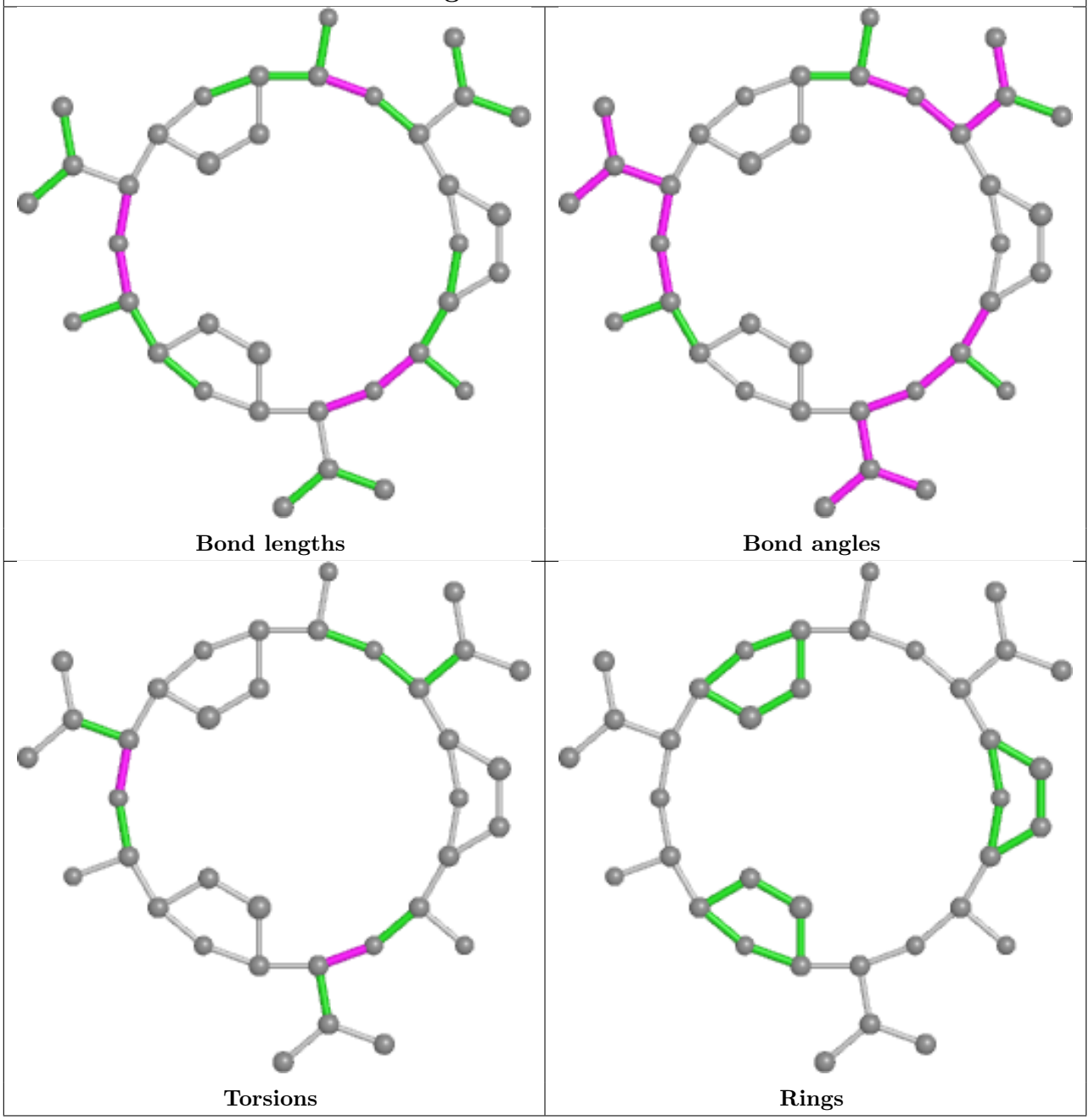
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6002	0JZ	10	0
2	A	6001	0JZ	12	0

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 0JZ B 6002



Ligand 0JZ A 6001



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	1182/1284 (92%)	-0.12	20 (1%)	70	61	118, 194, 243, 306	0
1	B	1182/1284 (92%)	-0.13	21 (1%)	68	59	123, 200, 243, 301	0
All	All	2364/2568 (92%)	-0.12	41 (1%)	70	61	118, 197, 244, 306	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	963	GLN	4.9
1	B	1199	THR	4.5
1	A	1084	ASP	4.0
1	A	574	GLU	3.9
1	B	228	TRP	3.7

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 monosaccharides in this entry.

6.4 Ligands (i)

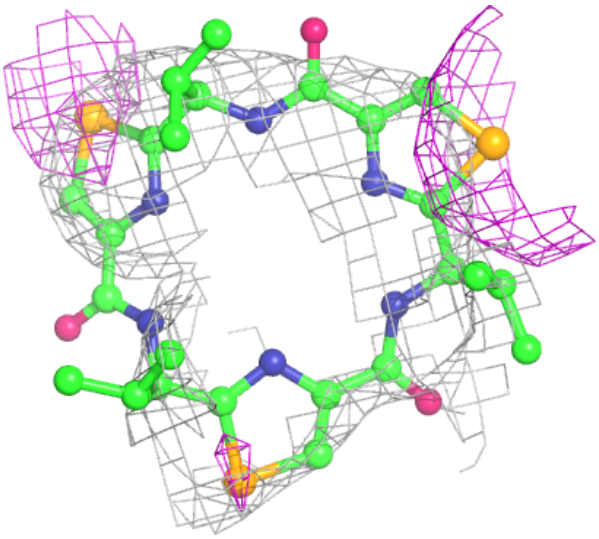
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

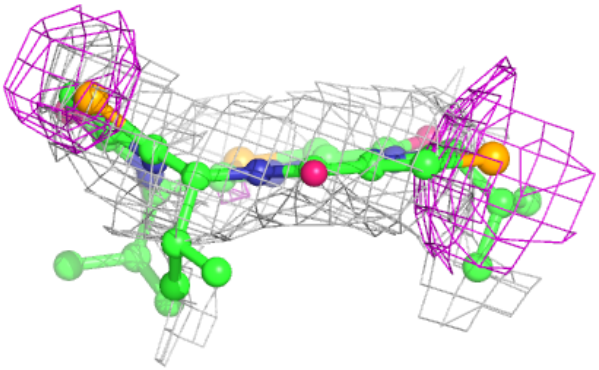
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	0JZ	B	6002	36/36	0.63	0.41	196,196,196,196	0
2	0JZ	A	6001	36/36	0.64	0.43	196,196,196,196	0

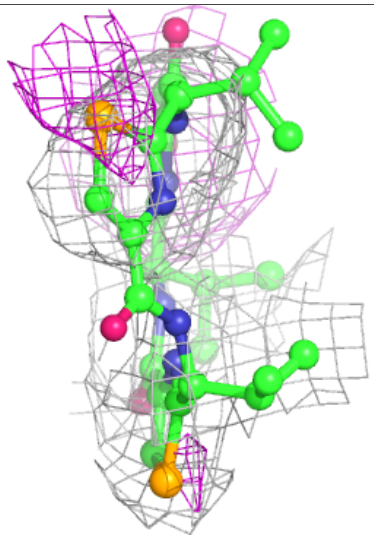
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 0JZ B 6002:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

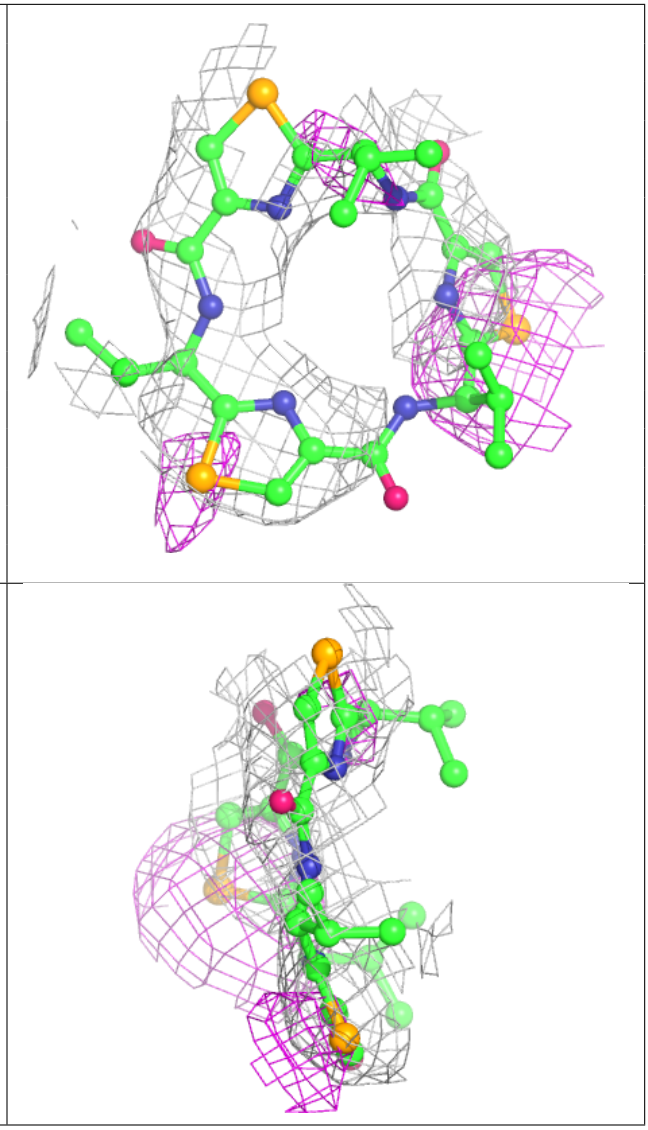






Electron density around 0JZ A 6001:

$2mF_o$-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.