wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:49 AM GMT

PDB ID	:	3G61
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	:	4.35 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 (1)) were used in the production of this report:

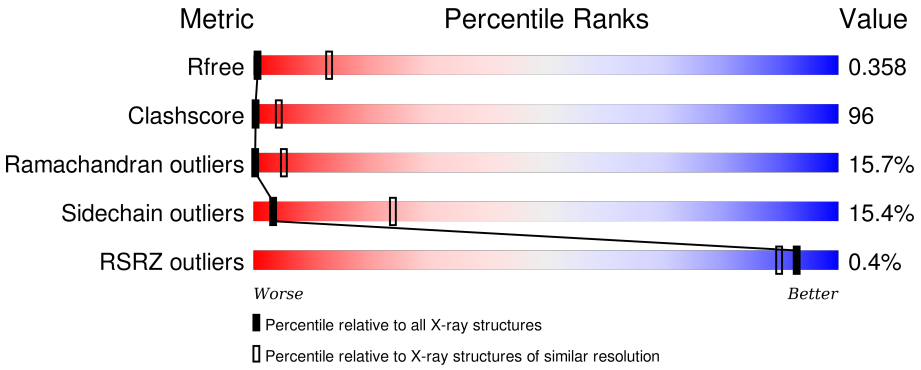
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 4.35 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}	91344	1063 (5.08-3.60)
Clashscore	102246	1171 (5.08-3.60)
Ramachandran outliers	100387	1110 (5.08-3.60)
Sidechain outliers	100360	1093 (5.08-3.60)
RSRZ outliers	91569	1067 (5.08-3.60)

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.

Mol	Chain	Length	Quality of chain
1	A	1284	13% 57% 19% • 8%
1	B	1284	12% 59% 19% • 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	2J8	A	6002	-	-	-	X
2	2J8	B	6003	-	-	-	X
2	2J8	B	6004	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18448 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.

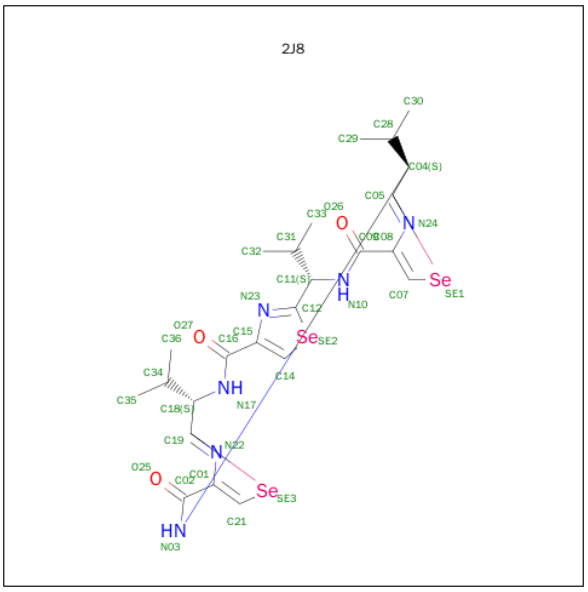
- Molecule 1 is a protein called Multidrug resistance protein 1a.

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

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 (4S,11S,18S)-4,11,18-TRI(PROPAN-2-YL)-6,13,20-TRISELENA-3,10,17,22,23,24-HEXAAZATETRACYCLO[17.2.1.1 5,8 .1 12,15]TETRACOSA-1(21),5(24),7,12(23),14,19(22)-HEXAENE-2,9,16-TRIONE (three-letter code: 2J8) (formula: $C_{24}H_{30}N_6O_3Se_3$).



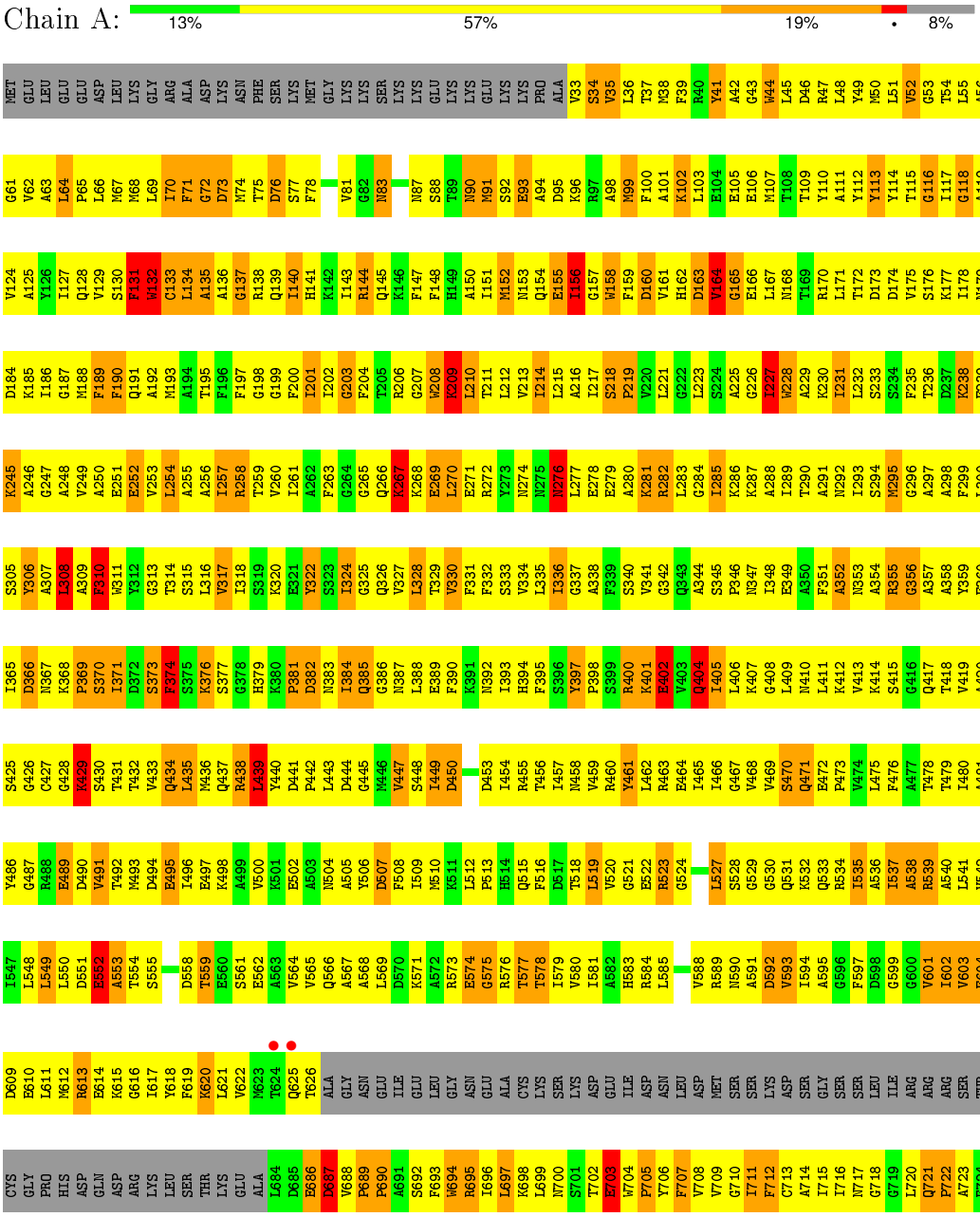
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		
2	A	1	Total	C	N	O	Se	0	0
			17	11	3	1	2		
2	B	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		
2	B	1	Total	C	N	O	Se	0	0
			17	11	3	1	2		

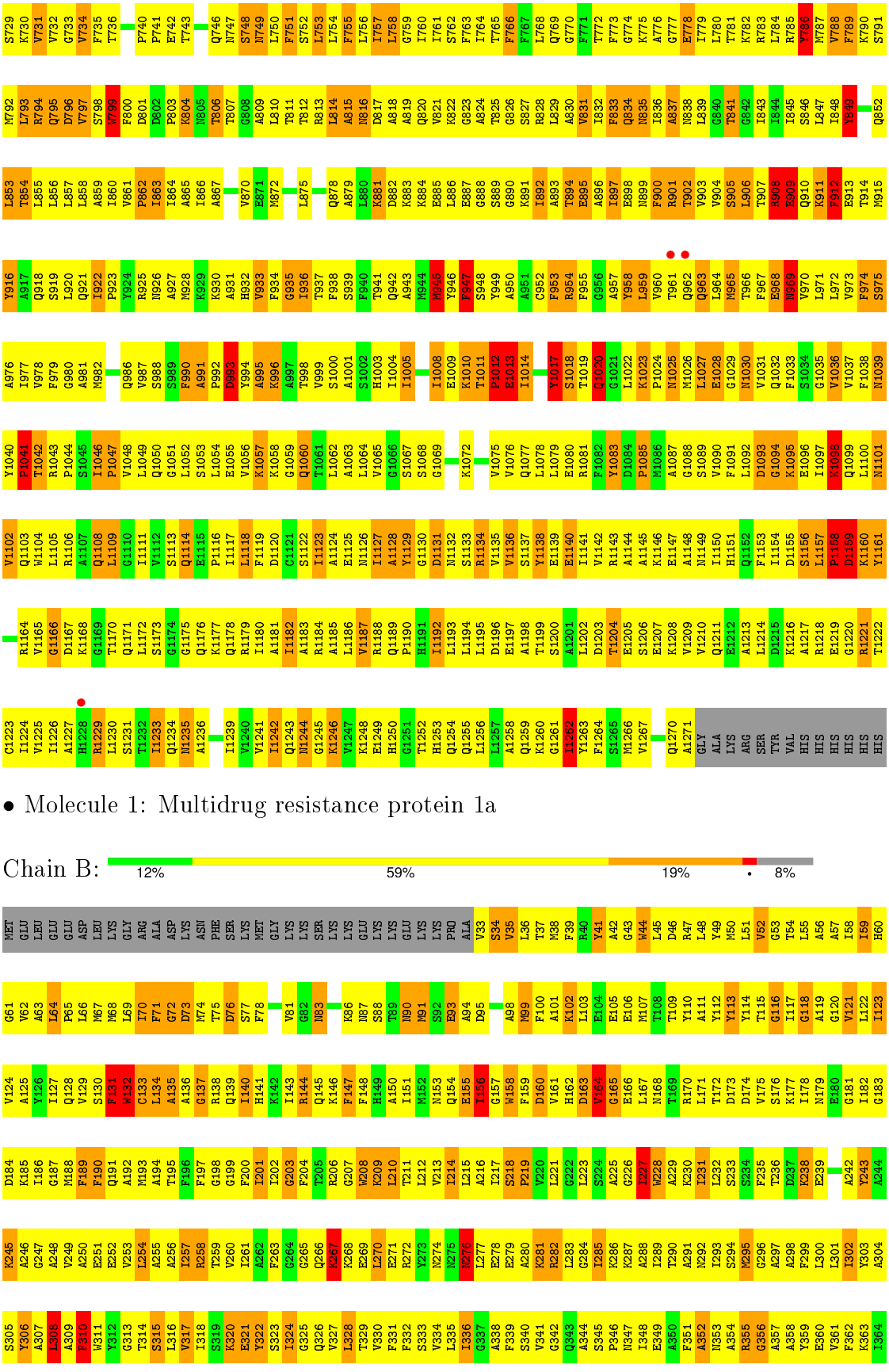
3 Residue-property plots (i)

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.

- Molecule 1: Multidrug resistance protein 1a

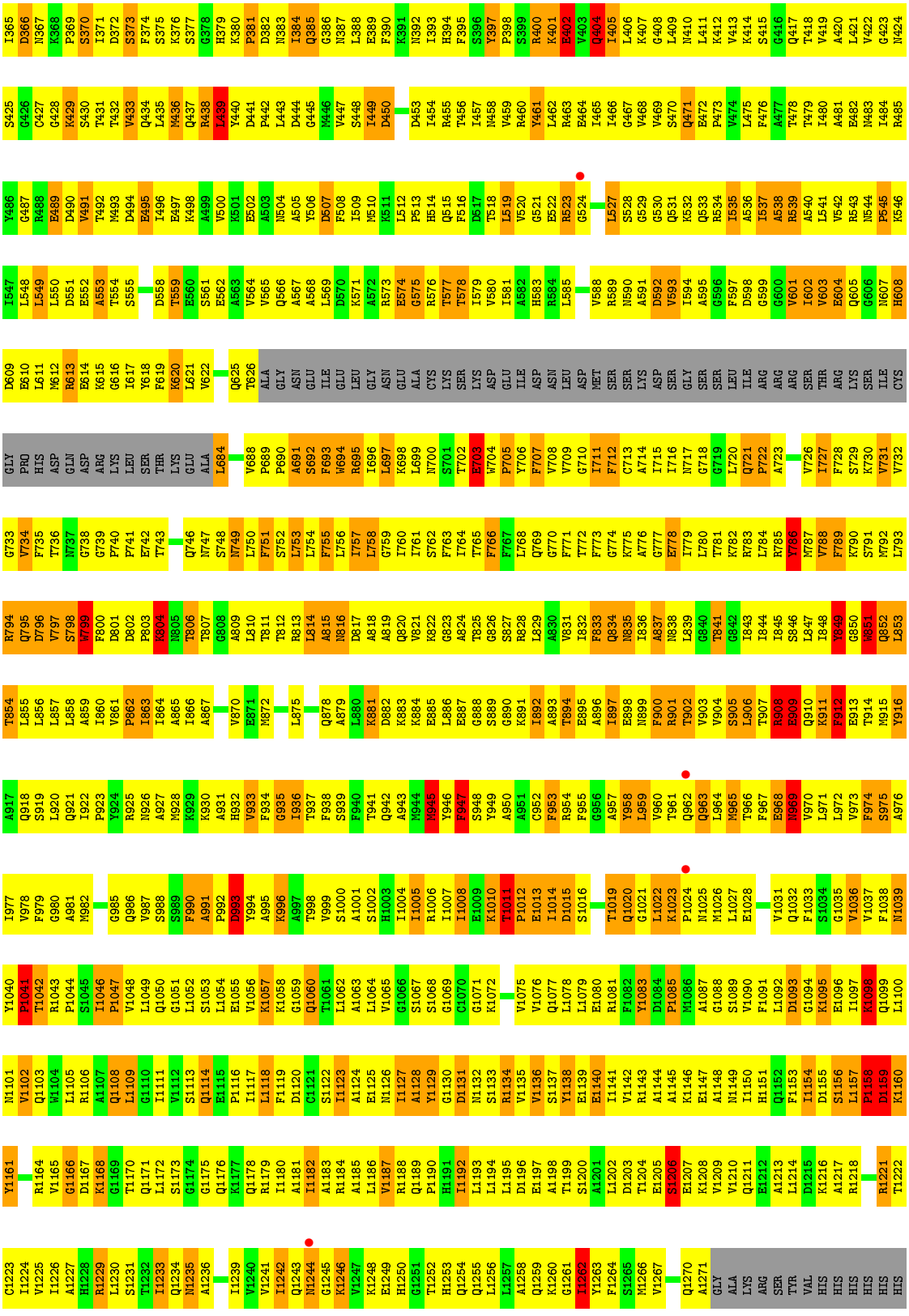
Chain A:





• Molecule 1: Multidrug resistance protein 1a

Chain B:


I365 D366 N367 K368 P369 S370 I371 D372 S373 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 Q434 L435 M436 Q437 R438 L439 Y440 D441 P442 L443 D444 G445 M446 V447 S448 I449 D450 D453 I454 R455 T456 I457 N458 V459 R460 Y461 L462 R463 E464 I465 I466 G467 V468 V469 S470 Q471 E472 P473 V474 L475 F476 A477 T478 T479 I480 A481 E482 N483 I484 R485
Y486 G487 R488 E489 D490 V491 T492 M493 D494 E495 I496 E497 K498 A499 V500 K501 E502 A503 N504 A505 Y506 D507 F508 I509 M510 K511 L512 P513 H514 Q515 F516 D517 T518 L519 V520 G521 E522 R523 G524 L527 S528 G529 G530 Q531 K532 Q533 R534 I535 A536 I537 A538 R539 A540 L541 I542 R543 N544 P545 K546
I547 L548 L549 L550 D551 E552 A553 T554 S555 D558 T559 E560 S561 E562 A563 V564 V565 Q566 A567 A568 L569 D570 K571 A572 R573 E574 G575 R576 T577 T578 I579 V580 I581 A582 H583 R584 L585 V588 R589 N590 A591 D592 V593 I594 A595 G596 F597 D598 G599 G600 V601 I602 V603 E604 Q605 G606 N607 H608
D609 E610 L611 M612 R613 E614 K615 G616 I617 Y618 F619 K620 L621 V622 Q625 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 V688 P689 P690 A691 S692 F693 W694 R695 I696 L697 K698 L699 N700 S701 T702 E703 W704 P705 Y706 F707 V708 V709 G710 I711 F712 C713 A714 I715 I716 N717 G718 G719 L720 Q721 P722 A723 V726 I727 F728 S729 K730 V731 V732
G733 V734 F735 T736 N737 G738 G739 P740 P741 E742 T743 Q746 N747 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 R785 Y786 M787 V788 F789 K790 S791 M792 L793
R794 Q795 D796 V797 S798 W799 F800 D801 D802 P803 K804 N805 T806 T807 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 Y849 G850 M851 Q852 L853
T854 L855 L856 L857 L858 A859 I860 V861 P862 I863 I864 A865 I866 A867 V870 E871 M872 L875 Q878 A879 L880 K881 D882 K883 K884 E885 L886 E887 G888 S889 G890 K891 I892 A893 T894 E895 A896 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 Y924 R925 N926 A927 M928 K929 K930 A931 H932 V933 F934 G935 I936 T937 F938 S939 F940 T941 Q942 A943 M944 M945 Y946 F947 S948 Y949 A950 A951 C952 F953 R954 F955 G956 A957 Y958 L959 V960 T961 D962 Q963 L964 M965 T966 F967 E968 N969 V970 L971 V972 V973 F974 S975 A976
I977 V978 F979 G980 A981 M982 G985 Q986 V987 S988 S989 F990 A991 P992 D993 Y994 A995 K996 A997 T998 V999 S1000 A1001 S1002 H1003 I1004 I1005 R1006 I1007 I1008 E1009 K1010 I1011 P1012 E1013 I1014 D1015 S1016 T1019 Q1020 G1021 L1022 K1023 P1024 N1025 M1026 L1027 E1028 V1031 Q1032 F1033 S1034 G1035 V1036 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 A1063 L1064 V1065 G1066 S1067 S1068 G1069 C1070 G1071 K1072 V1075 V1076 Q1077 L1078 L1079 E1080 R1081 F1082 Y1083 D1084 P1085 M1086 A1087 G1088 S1089 V1090 F1091 L1092 D1093 G1094 K1095 E1096 I1097 K1098 Q1099 L1100
N1101 V1102 Q1103 W1104 L1105 R1106 A1107 Q1108 L1109 G1110 I1111 V1112 S1113 Q1114 E1115 P1116 I1117 L1118 F1119 D1120 C1121 S1122 I1123 A1124 E1125 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 Q1152 F1153 I1154 D1155 S1156 L1157 P1158 D1159 K1160
Y1161 R1164 V1165 G1166 D1167 K1168 G1169 T1170 Q1171 L1172 S1173 G1174 G1175 Q1176 K1177 Q1178 R1179 I1180 A1181 I1182 A1183 R1184 A1185 L1186 V1187 R1188 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 R1221 T1222
C1223 I1224 V1225 I1226 A1227 H1228 R1229 L1230 S1231 T1232 I1233 Q1234 N1235 A1236 I1239 V1240 V1241 I1242 Q1243 N1244 G1245 K1246 V1247 K1248 E1249 H1250 G1251 T1252 H1253 Q1254 Q1255 L1256 L1257 A1258 Q1259 K1260 G1261 I1262 Y1263 F1264 S1265 N1266 V1267 Q1270 A1271 GLY ALA LYS ARG SER TYR VAL 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	97.74Å 114.98Å 375.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 4.35 19.95 – 4.35	Depositor EDS
% Data completeness (in resolution range)	93.3 (19.95-4.35) 93.2 (19.95-4.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.03 (at 4.36Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.308 , 0.356 0.312 , 0.358	Depositor DCC
R_{free} test set	2642 reflections (9.97%)	DCC
Wilson B-factor (Å^2)	195.7	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 28291 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18448	wwPDB-VP
Average B, all atoms (Å^2)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 2J8

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	0.40	0/9339	0.72	12/12626 (0.1%)
1	B	0.39	0/9339	0.71	14/12626 (0.1%)
All	All	0.40	0/18678	0.72	26/25252 (0.1%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	370	SER	N-CA-C	10.10	138.27	111.00
1	B	1159	ASP	N-CA-C	-8.41	88.29	111.00
1	A	374	PHE	N-CA-C	8.32	133.47	111.00
1	A	450	ASP	N-CA-C	-8.05	89.26	111.00
1	A	1098	LYS	N-CA-C	-7.76	90.04	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	916	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	916	TYR	Sidechain

5.2 Too-close contacts

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	1807	0
1	B	9171	0	9344	1791	0
2	A	53	0	36	5	0
2	B	53	0	36	20	0
All	All	18448	0	18760	3588	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 96.

The worst 5 of 3588 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:718:GLY:O	1:B:722:PRO:HD2	1.44	1.17
1:A:718:GLY:O	1:A:722:PRO:HD2	1.43	1.15
1:B:858:LEU:O	1:B:862:PRO:HD2	1.47	1.15
1:A:195:THR:HB	1:A:340:SER:HB2	1.27	1.14
1:B:35:VAL:HG23	1:B:36:LEU:H	1.13	1.11

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	685 (58%)	305 (26%)	188 (16%)	0 5
1	B	1178/1284 (92%)	678 (58%)	318 (27%)	182 (15%)	0 5
All	All	2356/2568 (92%)	1363 (58%)	623 (26%)	370 (16%)	0 5

5 of 370 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	52	VAL
1	A	88	SER
1	A	131	PHE
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%)	823 (84%)	153 (16%)	3 23
1	B	976/1065 (92%)	829 (85%)	147 (15%)	3 25
All	All	1952/2130 (92%)	1652 (85%)	300 (15%)	3 24

5 of 300 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1109	LEU
1	B	132	TRP
1	B	1041	PRO
1	A	1138	TYR
1	A	1262	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1235	ASN

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Mol	Chain	Res	Type
1	B	179	ASN
1	B	1108	GLN
1	A	1244	ASN
1	B	83	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

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	$\#\|Z\| > 2$
2	2J8	A	6001	-	27,39,39	1.40	3 (11%)	24,57,57	1.60	6 (25%)
2	2J8	A	6002	-	10,18,39	1.48	1 (10%)	9,24,57	1.61	2 (22%)
2	2J8	B	6003	-	27,39,39	1.45	3 (11%)	24,57,57	1.47	6 (25%)
2	2J8	B	6004	-	10,18,39	1.64	1 (10%)	9,24,57	1.81	3 (33%)

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	2J8	A	6001	-	-	0/24/48/48	0/0/4/4
2	2J8	A	6002	-	-	0/8/16/48	0/0/2/4
2	2J8	B	6003	-	-	0/24/48/48	0/0/4/4
2	2J8	B	6004	-	-	0/8/16/48	0/0/2/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6003	2J8	C02-N03	3.03	1.41	1.34
2	B	6003	2J8	C09-N10	3.49	1.42	1.34
2	A	6001	2J8	C09-N10	3.65	1.42	1.34
2	A	6001	2J8	C02-N03	3.67	1.42	1.34
2	A	6001	2J8	C16-N17	3.76	1.42	1.34

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	6003	2J8	C04-N03-C02	2.05	125.46	122.02
2	B	6003	2J8	C29-C28-C04	2.12	113.23	111.30
2	B	6004	2J8	C21-C01-N22	2.24	115.14	109.36
2	A	6001	2J8	C29-C28-C04	2.45	113.54	111.30
2	A	6002	2J8	C18-N17-C16	2.59	126.37	122.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6001	2J8	4	0
2	A	6002	2J8	1	0
2	B	6003	2J8	16	0
2	B	6004	2J8	4	0

5.7 Other polymers (i)

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

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	1182/1284 (92%)	-0.55	5 (0%)	93	90	115, 180, 210, 247	0
1	B	1182/1284 (92%)	-0.53	4 (0%)	94	92	97, 183, 214, 303	0
All	All	2364/2568 (92%)	-0.54	9 (0%)	93	90	97, 182, 212, 303	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1024	PRO	4.0
1	A	962	GLN	3.9
1	B	1244	ASN	2.8
1	A	1228	HIS	2.6
1	B	524	GLY	2.5

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	2J8	B	6004	17/36	0.52	0.47	3.60	185,185,185,185	0
2	2J8	A	6002	17/36	0.67	0.54	2.85	185,185,185,185	0
2	2J8	B	6003	36/36	0.69	0.44	2.80	185,185,185,185	0
2	2J8	A	6001	36/36	0.79	0.36	1.49	185,185,185,185	0

6.5 Other polymers (i)

There are no such residues in this entry.