wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2021 – 06:12 PM EDT

PDB ID	:	3G5U
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	:	3.80 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 following versions of software and data (see references (1)) were used in the production of this report:

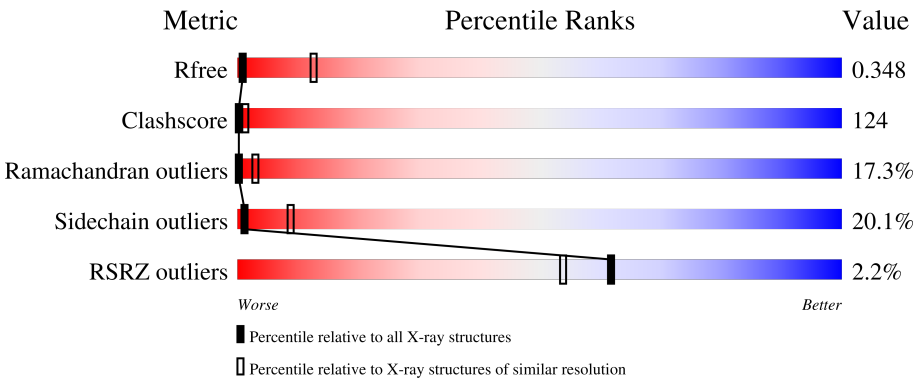
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.80 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))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 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% 11% 53% 24% • 8%
1	B	1284	2% 11% 55% 23% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18352 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	9170	5895	1552	1686	37	0	0	0
1	B	1182	9170	5895	1552	1686	37	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	952	ALA	CYS	engineered mutation	UNP Q5I1Y5
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	952	ALA	CYS	engineered mutation	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 MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
2	A	6	6	6	0	0

Continued on next page...

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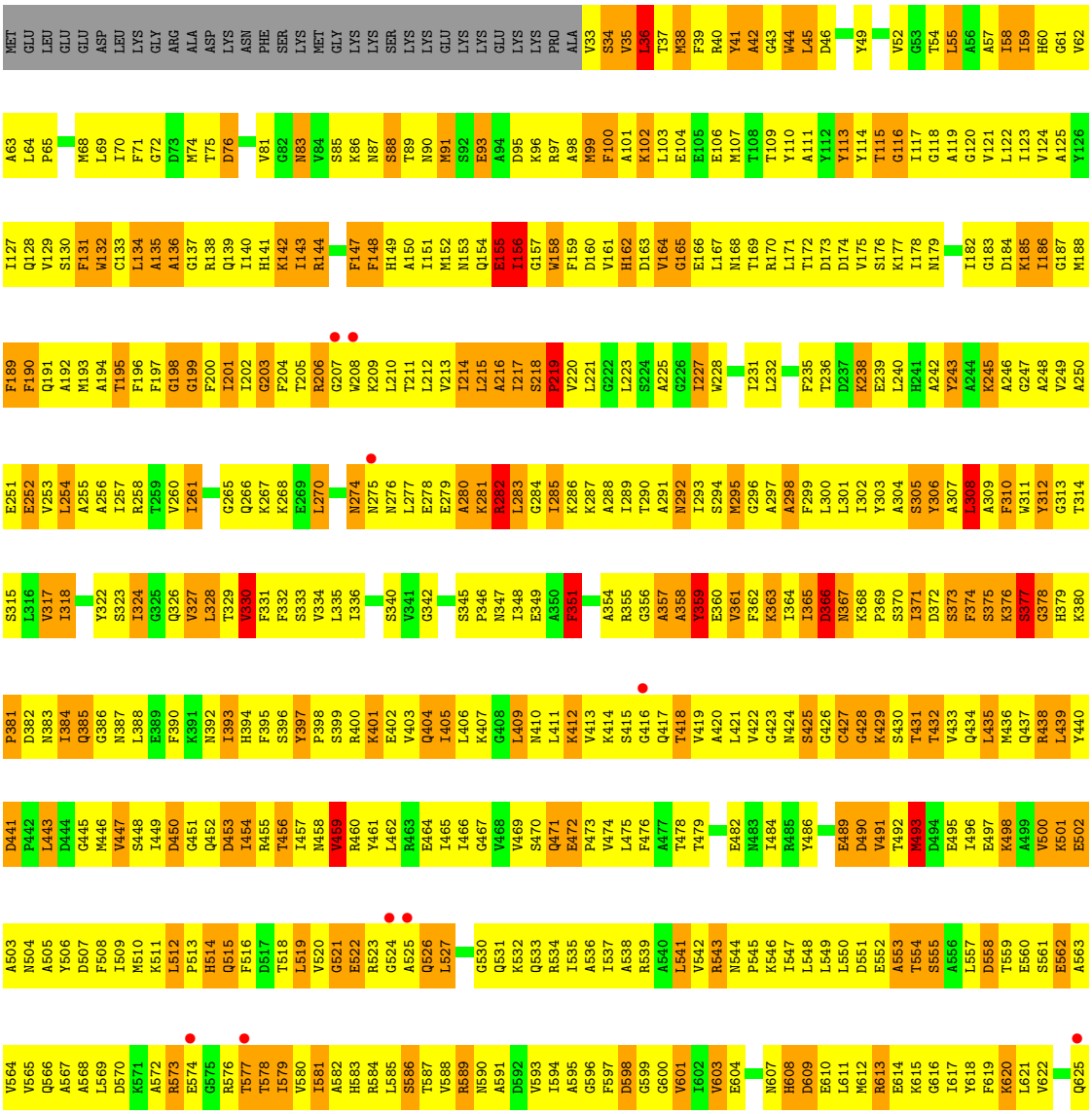
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
2	B	6	6	6	0	0

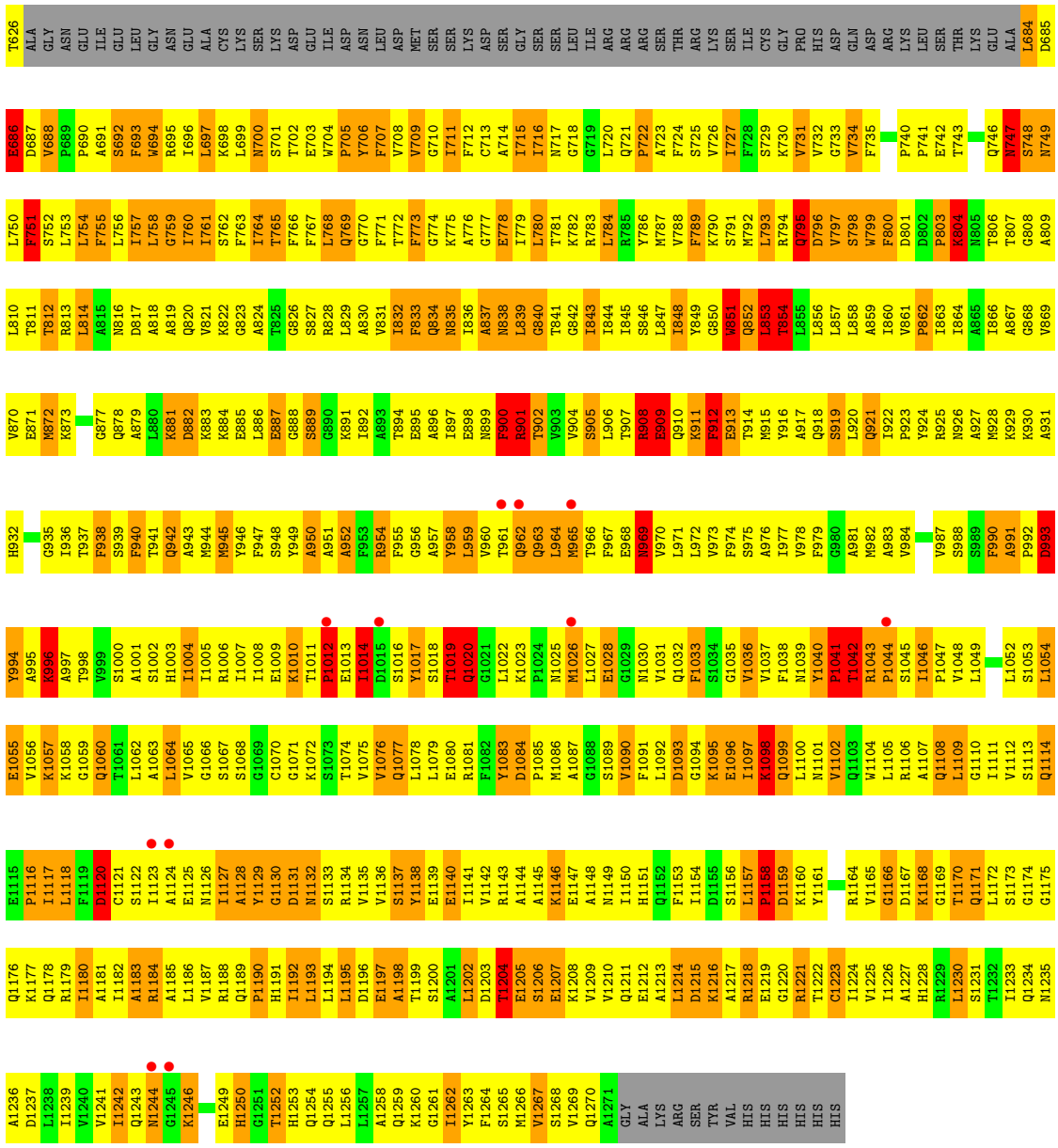
3 Residue-property plots (i)

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

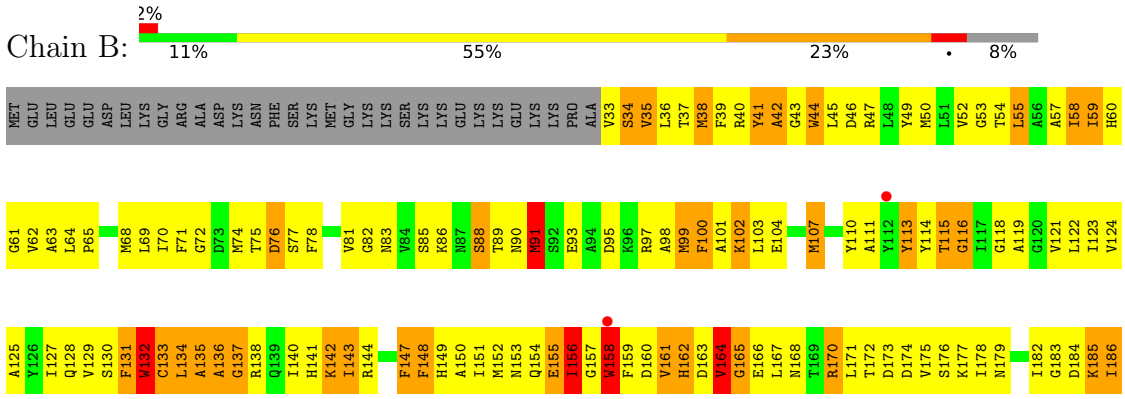
Chain A: 2% 11% 53% 24% 8%



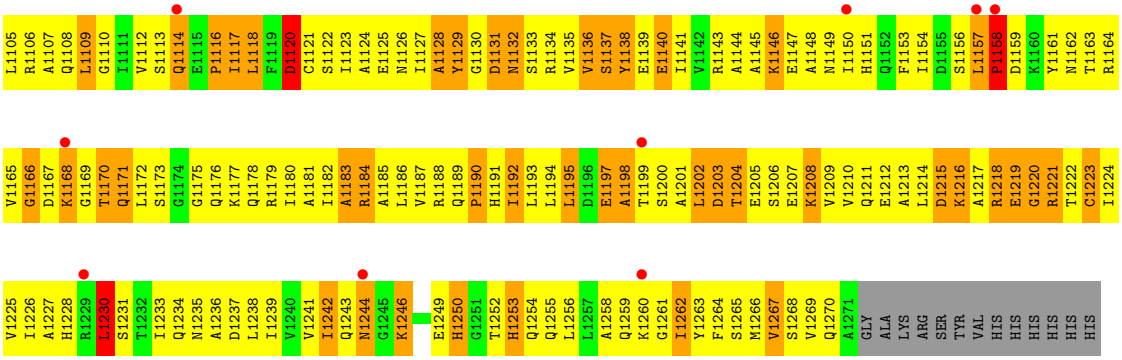


- Molecule 1: Multidrug resistance protein 1a

Chain B:



R1043 P1044 S1045 I1046 P1047 V1048 L1049 L1052 S1053 L1054 E1055 V1056 K1057 K1058 G1059 Q1060 T1061 L1062 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 V1090 F1091 L1092 D1093 G1094 K1095 E1096 I1097 K1098 Q1099 L1100 N1101 V1102 Q1103 W1104
M982 A983 V984 V987 S988 S989 F990 A991 P992 D993 Y994 A995 K996 A997 T998 V999 S1000 A1001 S1002 H1003 I1004 I1005 R1006 I1007 I1008 E1009 K1010 T1011 P1012 E1013 I1014 D1015 S1016 Y1017 S1018 T1019 Q1020 G1021 L1022 K1023 P1024 M1025 M1026 L1027 E1028 G1029 N1030 V1031 Q1032 F1033 S1034 G1035 V1036 V1037 F1038 N1039 Y1040 P1041 T1042
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 A952 F953 R954 F955 G956 A957 Y958 L959 V960 T961 Q962 Q963 L964 M965 T966 F967 E968 N969 V970 L971 L972 V973 T974 F974 S975 A976 I977 V978 F979 G980 A981
I860 V861 P862 I863 I864 A865 I866 A867 G868 V869 V870 E871 M872 K873 G877 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 P914 M915 Y916 A917 Q918 S919 L920 Q921
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 G826 S827 F766 F767 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
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 R828 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
LEU SER THR LYS GLU ALA L684 D685 E686 D687 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 F724 S725 V726 I727 F728 S729 K730 V731 V732 G733 V734 F735 T736 N737
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 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
A556 L557 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 S586 T587 V588 R589 N590 A591 D592 V593 T594 A595 G596 F597 D598 G599 G600 V601 I602 V603 E604 N607 H608 D609 E610 L611 M612 R613 E614 K615 G616
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 A525 Q526 L527 S528 G529 G530 Q531 K532 Q533 R534 I537 A538 L541 V542 R543 N544 P545 K546 I547 L548 L549 L550 D551 E552 A553 T554 S555
V433 Q434 L435 M436 Q437 R438 L439 Y440 D441 P442 L443 D444 G445 M446 V447 S448 I449 D450 G451 Q452 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 E482 N483 I484 R485 Y486 G487 R488 E489 D490 V491 T492 M493
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 M410 L411 K412 V413 K414 S415 G416 Q417 T418 V419 A420 L421 V422 G423 N424 S425 G426 C427 G428 K429 S430 T431 T432
F310 W311 Y312 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 A338 F339 S340 V341 G342 S345 P346 N347 I348 F351 A354 R355 G356 A357 A358 Y359 E360 V361 F362 K363 I364 I365 D366 N367 K368 P369 S370 I371 D372
S224 A225 G226 I227 W228 A229 K230 I231 L232 F235 T236 D237 K238 E239 L240 H241 A242 Y243 A244 K245 A246 G247
G187 M188 F189 F190 Q191 A192 M193 A194 T195 F196 F197 G198 G199 F200 I201 I202 G203 F204 T205 R206 G207 W208 K209 L210 T211 L212 V213 I214 L215 A216 I217 S218 P219 V220 L221 G222 L223
A248 V249 A250 E251 E252 V253 L254 A255 A256 I257 V260 I261 A262 F263 G264 G265 Q266 K267 K268 E269 L270 E271 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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A1107
Q1108
L1109
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V1112
S1113
Q1114
E1115
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F1119
D1120
C1121
S1122
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A1124
E1125
N1126
I1127
A1128
Y1129
G1130
D1131
N1132
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V1135
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E1140
I1141
V1142
R1143
A1144
A1145
K1146
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F1153
I1154
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N1162
T1163
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V1165
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T1170
Q1171
L1172
S1173
G1174
G1175
Q1176
K1177
Q1178
R1179
I1180
A1181
I1182
A1183
R1184
A1185
L1186
V1187
R1188
Q1189
P1190
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I1192
L1193
L1194
L1195
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E1212
A1213
L1214
D1215
K1216
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G1220
R1221
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C1223
I1224
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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	97.54Å 115.43Å 378.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.80 42.33 – 3.79	Depositor EDS
% Data completeness (in resolution range)	96.1 (19.98-3.80) 95.5 (42.33-3.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.19 (at 3.76Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.306 , 0.347 0.309 , 0.348	Depositor DCC
R_{free} test set	4245 reflections (10.21%)	wwPDB-VP
Wilson B-factor (Å^2)	132.2	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 113.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	18352	wwPDB-VP
Average B, all atoms (Å^2)	136.0	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: HG

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	0.54	1/9338 (0.0%)	0.88	22/12625 (0.2%)
1	B	0.51	0/9338	0.86	25/12625 (0.2%)
All	All	0.53	1/18676 (0.0%)	0.87	47/25250 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	600	GLY	CA-C	6.60	1.62	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	165	GLY	N-CA-C	-9.98	88.15	113.10
1	A	1097	ILE	N-CA-C	-8.94	86.87	111.00
1	A	994	TYR	N-CA-C	-8.30	88.59	111.00
1	A	1098	LYS	N-CA-C	-8.12	89.09	111.00
1	B	693	PHE	N-CA-C	7.98	132.54	111.00

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	9170	0	9338	2363	1
1	B	9170	0	9337	2245	1
2	A	6	0	0	0	0
2	B	6	0	0	0	0
All	All	18352	0	18675	4595	1

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 124.

The worst 5 of 4595 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:830:ALA:HB2	1:B:990:PHE:CE2	1.25	1.61
1:B:830:ALA:CB	1:B:990:PHE:CE2	2.06	1.36
1:B:830:ALA:CB	1:B:990:PHE:HE2	1.38	1.36
1:B:263:PHE:HE2	1:B:266:GLN:NE2	1.32	1.27
1:A:856:LEU:HD13	1:A:955:PHE:CD1	1.70	1.25

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:GLN:CG	1:B:450:ASP:OD1[1_455]	2.03	0.17

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%)	678 (58%)	299 (25%)	201 (17%)	0 3
1	B	1178/1284 (92%)	676 (57%)	295 (25%)	207 (18%)	0 2
All	All	2356/2568 (92%)	1354 (58%)	594 (25%)	408 (17%)	0 3

5 of 408 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	115	THR
1	A	135	ALA
1	A	156	ILE
1	A	164	VAL

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	975/1064 (92%)	775 (80%)	200 (20%)	1 8
1	B	975/1064 (92%)	783 (80%)	192 (20%)	1 9
All	All	1950/2128 (92%)	1558 (80%)	392 (20%)	1 9

5 of 392 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	206	ARG
1	B	577	THR
1	B	245	LYS
1	B	401	LYS
1	B	751	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	437	GLN
1	B	963	GLN
1	B	625	GLN
1	B	820	GLN
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)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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%)	-0.31	20 (1%)	70	62	36, 127, 195, 207	0
1	B	1182/1284 (92%)	-0.23	31 (2%)	56	47	47, 141, 200, 207	0
All	All	2364/2568 (92%)	-0.27	51 (2%)	62	54	36, 135, 198, 207	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	ASN	4.5
1	A	1244	ASN	4.3
1	B	382	ASP	4.3
1	A	961	THR	4.2
1	B	383	ASN	4.1

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	HG	A	1286	1/1	0.58	0.40	166,166,166,166	1
2	HG	B	1288	1/1	0.90	0.18	147,147,147,147	0
2	HG	A	1288	1/1	0.94	0.11	147,147,147,147	0
2	HG	B	1286	1/1	0.95	0.28	109,109,109,109	1
2	HG	B	1287	1/1	0.96	0.05	147,147,147,147	0
2	HG	A	1290	1/1	0.96	0.06	147,147,147,147	0
2	HG	B	1290	1/1	0.96	0.04	147,147,147,147	0
2	HG	A	1289	1/1	0.97	0.05	147,147,147,147	0
2	HG	B	1289	1/1	0.97	0.06	147,147,147,147	0
2	HG	B	1285	1/1	0.97	0.05	147,147,147,147	0
2	HG	A	1287	1/1	0.98	0.06	147,147,147,147	0
2	HG	A	1285	1/1	0.98	0.05	147,147,147,147	0

6.5 Other polymers (i)

There are no such residues in this entry.