



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:50 AM GMT

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

The following versions of software and data (see [references ⓘ](#)) 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

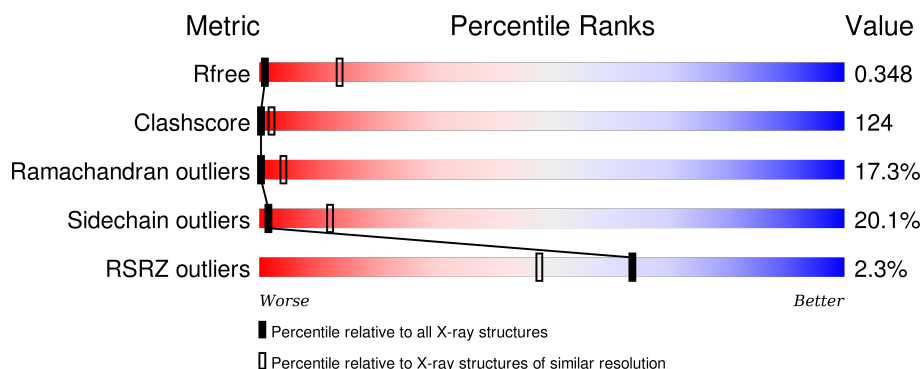
1 Overall quality at a glance

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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 $\leq 5\%$. 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

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
1	A	1182	Total	C	N	O	S	0	0	0
			9170	5895	1552	1686	37			
1	B	1182	Total	C	N	O	S	0	0	0
			9170	5895	1552	1686	37			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	952	ALA	CYS	ENGINEERED	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	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
2	B	6	Total	Hg	0	0
			6	6		

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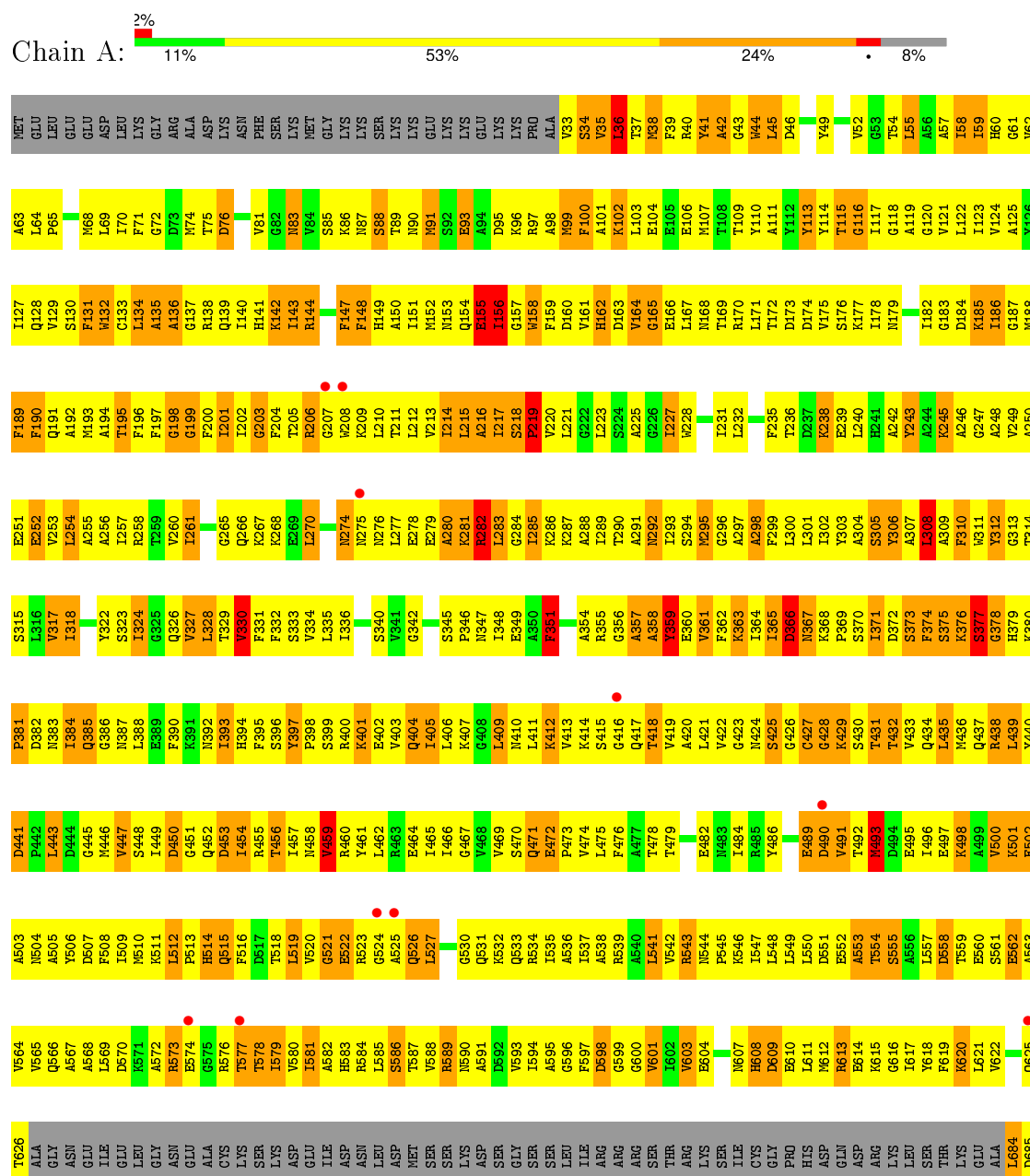
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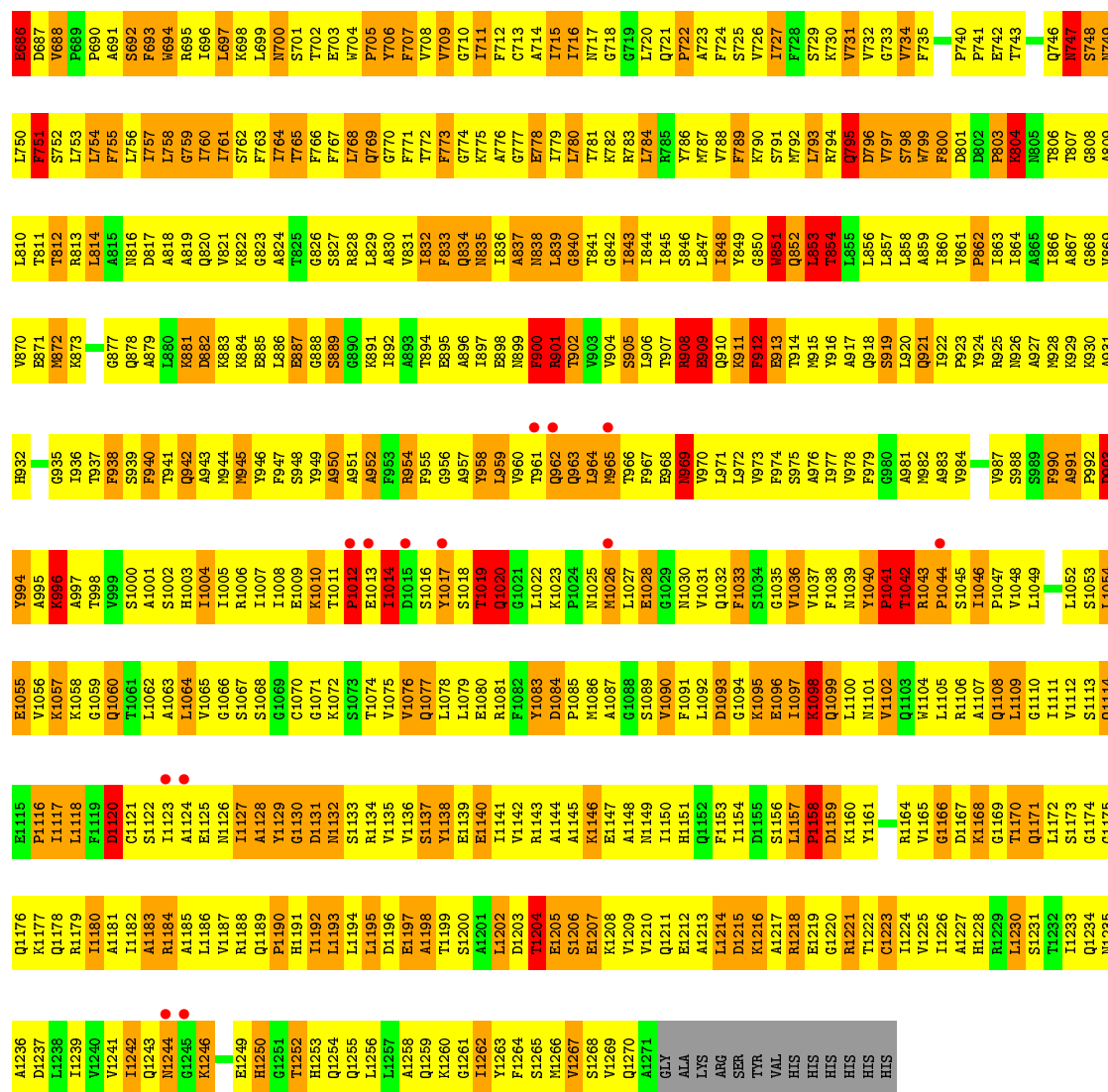
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Hg	0	0
			6	6		

3 Residue-property plots

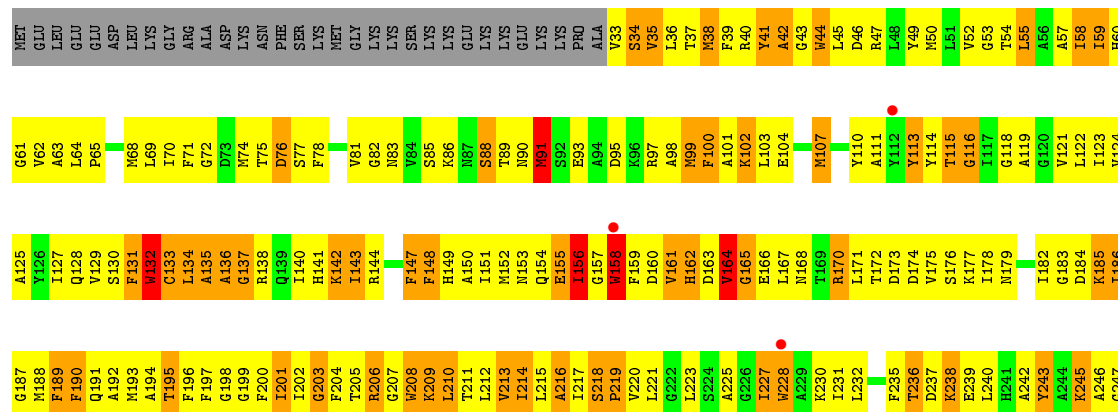
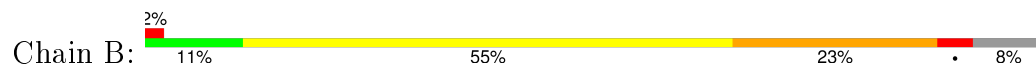
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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





• Molecule 1: Multidrug resistance protein 1a



L1105	R1043	M882	I860	W799	G738	LEU	I617	A556	D494	V433	S373	F310	A248
R1106	P1044	A983	V861	F800	G739	SER	Y618	L557	E495	Q434	F374	W311	V249
A1107	S1045	I862	I863	D801	P740	THR	F619	D558	I496	L436	S375	Y312	L450
Q1108	I1046	R925	R862	D802	P741	LYS	T559	K498	K499	M436	K376	G313	E251
L1109	P1047	N926	I864	P803	P742	GLU	L621	S560	K499	Q437	S377	T314	E252
G1110	V1048	N927	A865	K804	T743	ALA	V622	E561	A499	R438	G378	S315	V253
I1111	L1049	N928	I866	N805		L684		E562	V600	L439	R379	I316	L254
V1112		K929	A867	T806		D885	Q625	A563	K501	I440	R380	V317	A255
S1113	L1052	R930	G868	T807	N747	D886	T626	V564	E502	D441	P381	I318	A256
Q1114	S1053	A991	R869	R807	N748	D887	GLY	P442	A503	L443	R382	S319	
E1115	L1054	R932	V870	G808	S748	D888	ALA	Q566	N504	K320	R383	G319	
P1116	E1055	Y994	R871	A809	N749	V688	ASN	A567	A505	D444	I384	E321	
I1117	V1056	V933	M872	L810	L750	P689	GLU	A568	Y506	G445	Q385	Y322	
L1118	K1057	G935	K873	T812	S752	A891	ILE	L569	D507	M446	G386	S323	
F1119	K1058	A997		R813	L753	S692	GLU	D570	F508	V447	N387	I324	
D1120	G1059	T937	G877	L814	L754	F683	LEU	K571	I509	S448	L388	Q326	
C1121	Q1060	F938	K878	A815	F755	H694	GLY	A572	M510	I449	G325	G264	
S1122	S1000	S939	A879	N816	L756	R695	ASN	R573	F390	D450	F390	V327	
I1123	L1062	F940	L880	D817	L757	I696	GLU	E574	K511	G451	K391	L328	
A1124	A1063	T941	K881	A818	L758	L697	ALA	G575	P513	G452	N392	T329	
E1125	H1003	Q942	D882	A819	G759	K698	CYS	R576	H514	D453	I393	K330	
N1126	V1065	N943	K883	Q820	L760	L699	LYS	T577	Q515	L454	H394	F331	
I1127	G1066	N944	K884	V821	I761	N700	SER	T578	F516	R455	F395	F332	
A1128	S1067	N945	E885	K822	S762	S701	LYS	I579	D517	T456	S396	S333	
Y1129	S1068	Y946	L886	G823	F763	T702	ASP	V580	T518	I457	Y397	V334	
G1130	G1069	F947	E887		I764	E703	GLU	I581	L519	V458	P398	L335	
D1131	C1070	S948	G888	G826	T765	W704	ILE	A582	V520	V459	S399	N275	
N1132	G1071	Y949	S827	S827	F766	W705	ASP	H583	G521	R460	R400	N276	
S1133	S1072	A950	G890	R828	F767	Y706	ASN	R584	E522	Y461	K401	G337	
R1134	S1073	A951	K891	L829	L768	F707	LEU	L585	R523	L462	E202	F339	
V1135	E1013	A952	I892	A830	Q769	V708	ASP	S586	G524	R463	V403	E279	
I1136	V1075	F953	A893	V831	G770	V709	MET	T587	A535	E464	Q404	K281	
S1137	V1076	R954	I894	I832	F771	G710	SER	V588	Q526	L465	I405	R282	
E1138	S1016	F955	E895	F833	T772	I711	SER	R589	L527	T466	L406	L283	
I1139	Y1017	G956	A896	Q834	F773	L712	LYS	N590	S528	G467	K407	G284	
E1140	L1079	A957	I897	N835	G774	C713	ASP	A591	G529	V468	G408	I285	
I1141	T1019	Y958	E898	I836	K775	A714	SER	D592	G530	V469	L409	N347	
V1142	Q1020	L959	R899	A837	A776	I715	GLY	V593	Q531	S470	M410	I348	
R1143	F1082	T961	F900	N838	G777	I716	SER	I594	K532	Q471	L411		
A1144	Y1083	T961	R901	L839	E778	N717	SER	A595	Q533	E472	K412	I289	
A1145	K1023	Q962	T902	G840	L779	G718	LEU	G596	R534	P473	V413	T290	
K1146	P1024	Q963	V903	T841	L780	G719	ILE	F597	I537	V474	K414	A291	
E1147	M1025	L964	S904	G842	T781	L720	ARG	D598	A538	L475	S415	N292	
A1148	M1026	N965	S905	I843	K782	Q721	ARG	G599		T476	G416	I293	
N1149	L1027	T966	L906	I844	K783	P722	ARG	G600		A477	Q417	S294	
I1150	E1028	F967	T907	I845	L784	A723	SER	V601	L541	T479	T418	M295	
H1151	G1029	E968	R908	S846	R785	F724	THR	I602	V542	R543	V419	G296	
F1153	L1032	N969	Q909	L847	Y786	S725	ARG	V603	R543	A420	E360	A297	
I1154	Q1032	L971	K911	I848	M787	V726	LYS	E604	N544	L421	V361	A298	
D1155	F1033	L972	F912	G850	F789	I727	SER		P545	V422	F362	F299	
S1156	S1034	V973	E913	Q851	K790	F728	ILE	M607	K546	I484	K363	L300	
L1157	G1035	F974	T914	Q852	S791	S729	CYS	H608	I547	R485	I364	L301	
P1158	V1036	S975	M915	L853	M792	K730	GLY	D609	L548	Y486	I365	I302	
D1159	Q1099	A976	Y916	T854	L793	V731	PRO	E610	L549	G487	D866	Y303	
K1160	F1038	L977	L855	R794	K733	HIS	ASP	L611	L550	R488	N367	A304	
Y1161	L1100	N978	Q918	Q795	V734	G733	GLN	M612	D551	E489	G428	S305	
N1162	N1039	F979	Q918	L856	V734	G733	GLN	R613	E552	D490	K429	Y306	
T1163	Y1040	F979	S919	L857	D796	F735	ASP	E614	A553	V491	S370	A307	
R1164	V1102	G980	L920	L858	V797	T736	ARG	T554	T554	T492	T431	L308	
	W1104	T1042	Q921	A859	S798	N737	LYS	G616	S555	V493	T432	A309	

V1165	G1166	D1167	K1168	T1169	Q1170	Q1171	L1172	S1173	G1174	Q1175	Q1176	K1177	Q1178	R1179	I1180	A1181	I1182	A1183	R1184	A1185	L1186	V1187	R1188	Q1189	F1190	H1191	I1192	L1193	L1194	L1195	D1196	E1197	A1198	T1199	S1200	A1201	L1202	D1203	T1204	E1205	S1206	E1207	K1208	V1209	Q1210	E1211	E1212	A1213	L1214	D1215	K1216	A1217	R1218	E1219	G1220	R1221	T1222	G1223	I1224
V1225	I1226	A1227	H1228	R1229	L1230	S1231	T1232	I1233	Q1234	N1235	A1236	D1237	L1238	I1239	V1240	V1241	I1242	Q1243	N1244	G1245	K1246	E1249	H1250	G1251	T1252	H1253	Q1254	Q1255	L1256	L1257	A1258	Q1259	K1260	G1261	I1262	Y1263	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

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
$\langle I/\sigma(I) \rangle$ 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	4203 reflections (10.22%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 41573 reflections (0.002%)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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(°)	Ideal(°)
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 ⓘ

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	4
1	B	1178/1284 (92%)	676 (57%)	295 (25%)	207 (18%)	0	3
All	All	2356/2568 (92%)	1354 (58%)	594 (25%)	408 (17%)	0	4

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 ⓘ

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	11
1	B	975/1064 (92%)	783 (80%)	192 (20%)	1	13
All	All	1950/2128 (92%)	1558 (80%)	392 (20%)	1	12

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

Mol	Chain	Res	Type
1	A	1108	GLN
1	B	147	PHE
1	B	1054	LEU
1	A	1140	GLU
1	A	1267	VAL

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

Mol	Chain	Res	Type
1	A	1235	ASN
1	B	141	HIS
1	B	1099	GLN
1	A	1244	ASN
1	B	83	ASN

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](#)

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%)	-0.28	23 (1%) 70 54	36, 127, 195, 207	0
1	B	1182/1284 (92%)	-0.20	32 (2%) 58 42	47, 141, 200, 207	0
All	All	2364/2568 (92%)	-0.24	55 (2%) 64 48	36, 135, 198, 207	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	ASN	4.6
1	A	1244	ASN	4.4
1	B	382	ASP	4.4
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 carbohydrates 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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	HG	B	1287	1/1	0.96	0.05	-1.87	147,147,147,147	0
2	HG	A	1287	1/1	0.98	0.06	-2.43	147,147,147,147	0
2	HG	A	1290	1/1	0.96	0.06	-2.66	147,147,147,147	0
2	HG	B	1290	1/1	0.96	0.04	-3.30	147,147,147,147	0
2	HG	B	1289	1/1	0.97	0.06	-	147,147,147,147	0
2	HG	A	1289	1/1	0.97	0.05	-	147,147,147,147	0
2	HG	B	1285	1/1	0.97	0.05	-	147,147,147,147	0
2	HG	B	1288	1/1	0.90	0.18	-	147,147,147,147	0
2	HG	A	1285	1/1	0.98	0.05	-	147,147,147,147	0
2	HG	A	1286	1/1	0.58	0.40	-	166,166,166,166	1
2	HG	B	1286	1/1	0.95	0.28	-	109,109,109,109	1
2	HG	A	1288	1/1	0.94	0.11	-	147,147,147,147	0

6.5 Other polymers [i](#)

There are no such residues in this entry.