



wwPDB X-ray Structure Validation Summary Report ⓘ

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)

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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

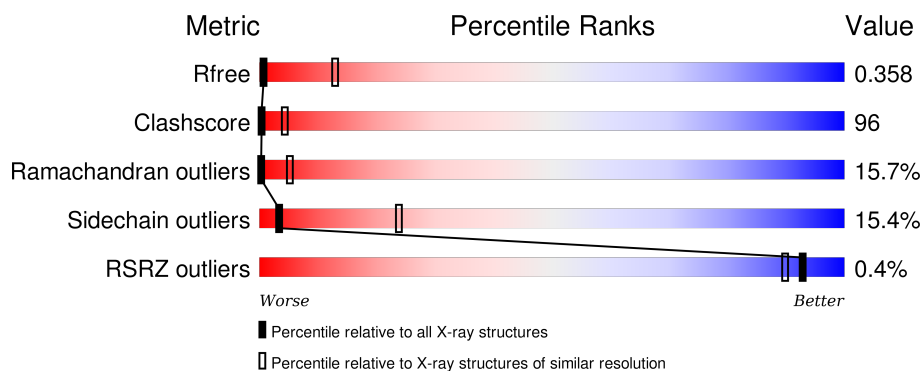
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

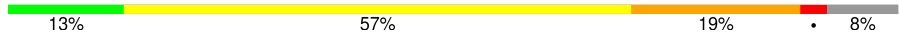
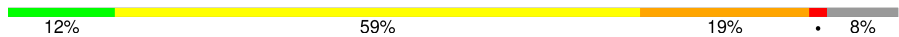
The reported resolution of this entry is 4.35 Å.

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 $\leq 5\%$. 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	
1	B	1284	

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.

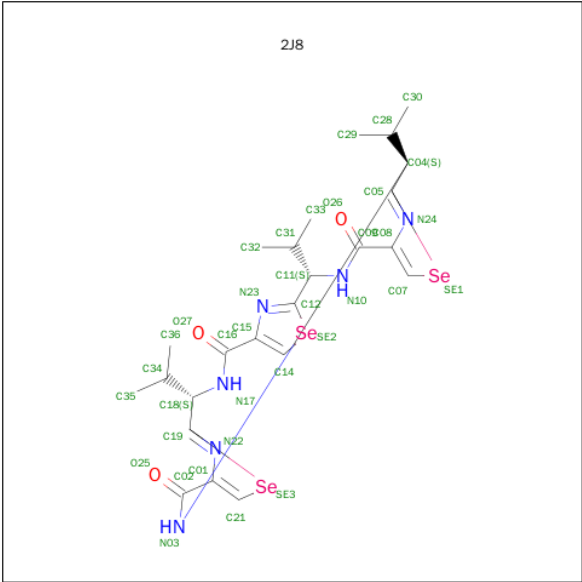
- Molecule 1 is a protein called Multidrug resistance protein 1a.

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: C₂₄H₃₀N₆O₃Se₃).



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		

S729	W792	L853	Y916	A976	Y1040	V1102	R164	G1223	G1159	Q1108	A1107	L1108	Q1109	Q1110	V1048	P1047	L1046	P1045	Q921	L858	W797	G734	V732	L731	K730	S729
K730	L793	L854	A917	I977	P1041	Q1103	V1166	I1224	R1229	Q1108	A1107	Q1109	Q1110	V1048	P1047	L1046	P1045	Q921	L858	W797	G734	V732	L731	K730	S729	
L793	L794	L855	Q918	Y978	T1042	W1104	V1166	I1225	R1229	Q1108	A1107	Q1109	Q1110	V1048	P1047	L1046	P1045	Q921	L858	W797	G734	V732	L731	K730	S729	
L794	L795	L856	Q919	Y979	T1043	W1105	V1167	I1226	R1230	Q1109	A1108	Q1110	Q1111	V1049	P1048	L1047	P1046	Q922	L859	W798	G735	V733	L732	K731	S730	
L795	L796	L857	Q920	Y980	T1044	W1106	V1168	I1227	R1231	Q1110	A1109	Q1111	Q1112	V1050	P1049	P1048	P1047	Q923	L860	W799	G736	V734	L733	K732	S731	
L796	L797	L858	Q921	Y981	T1045	W1107	V1169	I1228	R1232	Q1111	A1110	Q1112	Q1113	V1051	P1050	P1049	P1048	Q924	L861	W800	G737	V735	L734	K733	S732	
L797	L798	L859	Q922	Y982	T1046	W1108	V1170	I1229	R1233	Q1112	A1111	Q1113	Q1114	V1052	P1051	P1050	P1049	Q925	L862	W801	G738	V736	L735	K734	S733	
L798	L799	L860	Q923	Y983	T1047	W1109	V1171	I1230	R1234	Q1113	A1112	Q1114	Q1115	V1053	P1052	P1051	P1050	Q926	L863	W802	G739	V737	L736	K735	S734	
L799	L800	L861	Q924	Y984	T1048	W1110	V1172	I1231	R1235	Q1114	A1113	Q1115	Q1116	V1054	P1053	P1052	P1051	Q927	L864	W803	G740	V738	L737	K736	S735	
L800	L801	L862	Q925	Y985	T1049	W1111	V1173	I1232	R1236	Q1115	A1114	Q1116	Q1117	V1055	P1054	P1053	P1052	Q928	L865	W804	G741	V739	L738	K737	S736	
L801	L802	L863	Q926	Y986	T1050	W1112	V1174	I1233	R1237	Q1116	A1115	Q1117	Q1118	V1056	P1055	P1054	P1053	Q929	L866	W805	G742	V740	L739	K738	S737	
L802	L803	L864	Q927	Y987	T1051	W1113	V1175	I1234	R1238	Q1117	A1116	Q1118	Q1119	V1057	P1056	P1055	P1054	Q930	L867	W806	G743	V741	L740	K739	S738	
L803	L804	L865	Q928	Y988	T1052	W1114	V1176	I1235	R1239	Q1118	A1117	Q1119	Q1120	V1058	P1057	P1056	P1055	Q931	W807	W807	G744	V742	L741	K740	S739	
L804	L805	L866	Q929	Y989	T1053	W1115	V1177	I1236	R1240	Q1119	A1118	Q1120	Q1121	V1059	P1058	P1057	P1056	Q932	W808	W808	G745	V743	L742	K741	S740	
L805	L806	L867	Q930	Y990	T1054	W1116	V1178	I1237	R1241	Q1120	A1119	Q1121	Q1122	V1060	P1059	P1058	P1057	Q933	W809	W809	G746	V744	L743	K742	S741	
L806	L807	L868	Q931	Y991	T1055	W1117	V1179	I1238	R1242	Q1121	A1120	Q1122	Q1123	V1061	P1060	P1059	P1058	Q934	W810	W810	G747	V745	L744	K743	S742	
L807	L808	L869	Q932	Y992	T1056	W1118	V1180	I1239	R1243	Q1122	A1121	Q1123	Q1124	V1062	P1061	P1060	P1059	Q935	W811	W811	G748	V746	L745	K744	S743	
L808	L809	L870	Q933	Y993	T1057	W1119	V1181	I1240	R1244	Q1123	A1122	Q1124	Q1125	V1063	P1062	P1061	P1060	Q936	W812	W812	G749	V747	L746	K745	S744	
L809	L810	L871	Q934	Y994	T1058	W1120	V1182	I1241	R1245	Q1124	A1123	Q1125	Q1126	V1064	P1063	P1062	P1061	Q937	W813	W813	G750	V748	L747	K746	S745	
L810	L811	L872	Q935	Y995	T1059	W1121	V1183	I1242	R1246	Q1125	A1124	Q1126	Q1127	V1065	P1064	P1063	P1062	Q938	W814	W814	G751	V749	L748	K747	S746	
L811	L812	L873	Q936	Y996	T1060	W1122	V1184	I1243	R1247	Q1126	A1125	Q1127	Q1128	V1066	P1065	P1064	P1063	Q939	W815	W815	G752	V750	L749	K748	S747	
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L815	L816	L877	Q940	Y1000	T1064	W1126	V1188	I1247	R1251	Q1130	A1129	Q1131	Q1132	V1070	P1069	P1068	P1067	Q943	W819	W819	G756	V754	L753	K752	S751	
L816	L817	L878	Q941	Y1001	T1065	W1127	V1189	I1248	R1252	Q1131	A1130	Q1132	Q1133	V1071	P1070	P1069	P1068	Q944	W820	W820	G757	V755	L754	K753	S752	
L817	L818	L879	Q942	Y1002	T1066	W1128	V1190	I1249	R1253	Q1132	A1131	Q1133	Q1134	V1072	P1071	P1070	P1069	Q945	W821	W821	G758	V756	L755	K754	S753	
L818	L819	L880	Q943	Y1003	T1067	W1129	V1191	I1250	R1254	Q1133	A1132	Q1134	Q1135	V1073	P1072	P1071	P1070	Q946	W822	W822	G759	V757	L756	K755	S754	
L819	L820	L881	Q944	Y1004	T1068	W1130	V1192	I1251	R1255	Q1134	A1133	Q1135	Q1136	V1074	P1073	P1072	P1071	Q947	W823	W823	G760	V758	L757	K756	S755	
L820	L821	L882	Q945	Y1005	T1069	W1131	V1193	I1252	R1256	Q1135	A1134	Q1136	Q1137	V1075	P1074	P1073	P1072	Q948	W824	W824	G761	V759	L758	K757	S756	
L821	L822	L883	Q946	Y1006	T1070	W1132	V1194	I1253	R1257	Q1136	A1135	Q1137	Q1138	V1076	P1075	P1074	P1073	Q949	W825	W825	G762	V760	L759	K758	S757	
L822	L823	L884	Q947	Y1007	T1071	W1133	V1195	I1254	R1258	Q1137	A1136	Q1138	Q1139	V1077	P1076	P1075	P1074	Q950	W826	W826	G763	V761	L760	K759	S758	
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L824	L825	L886	Q949	Y1009	T1073	W1135	V1197	I1256	R1260	Q1139	A1138	Q1140	Q1141	V1079	P1078	P1077	P1076	Q952	W828	W828	G765	V763	L762	K761	S760	
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L827	L828	L889	Q952	Y1012	T1076	W1138	V1200	I1259	R1263	Q1142	A1141	Q1143	Q1144	V1082	P1081	P1080	P1079	Q955	W831	W831	G768	V766	L765	K764	S763	
L828	L829	L890	Q953	Y1013	T1077	W1139	V1201	I1260	R1264	Q1143	A1142	Q1144	Q1145	V1083	P1082	P1081	P1080	Q956	W832	W832	G769	V767	L766	K765	S764	
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L833	L834	L895	Q958	Y1018	T1082	W1144	V1206	I1265	R1269	Q1148	A1147	Q1149	Q1150	V1088	P1087	P1086	P1085	Q961	W837	W837	G774	V772	L771	K770	S769	
L834	L835	L896	Q959	Y1019	T1083	W1145	V1207	I1266	R1270	Q1149	A1148	Q1150	Q1151	V1089	P1088	P1087	P1086	Q962	W838	W838	G775	V773	L772	K771	S770	
L835	L836	L897	Q960	Y1020	T1084	W1146	V1208	I1267	R1271	Q1150	A1149	Q1151	Q1152	V1090	P1089	P1088	P1087	Q963	W839	W839	G776	V774	L773	K772	S771	
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L838	L839	L900	Q963	Y1023	T1087	W1149	V1211	I1270	R1274	Q1153	A1152	Q1154	Q1155	V1093	P1092	P1091	P1090	Q966	W842	W842	G779	V777	L776	K775	S774	
L839	L840	L901	Q964	Y1024	T1088	W1150	V1212	I1271	R1275	Q1154	A1153	Q1155	Q1156	V1094	P1093	P1092	P1091	Q967	W843	W843	G780	V778	L777	K776	S775	
L840	L841	L902	Q965	Y1025	T1089	W1151	V1213	I1272	R1276	Q1155	A1154	Q1156	Q1157	V1095	P1094	P1093	P1092	Q968	W844	W844	G781	V779	L778	K777	S776	
L841	L842	L903	Q966	Y1026	T1090	W1152	V1214	I1273	R1277	Q1156	A1155	Q1157	Q1158	V1096	P1095	P1094	P1093	Q969	W845	W845	G782	V780	L779	K778	S777	
L842	L843	L904	Q967	Y1027	T1091	W1153	V1215	I1274	R1278	Q1157	A1156	Q1158	Q1159	V1097	P1096	P1095	P1094	Q970	W846	W846	G783	V781	L780	K779	S778	
L843	L844	L905	Q968	Y1028	T1092	W1154	V																			

G1223	Y1161	H1101	Y1040	I977	A917	T854	R794	G733	GLY	D609	I547	Y486	S425	I365
I1224		Y1102	P1041	V978	Q918	L855	Q795	V734	PRO	E610	L548	G487	G426	D866
V1225	R1164	Y1103	T1042	F979	S919	L856	D796	F735	HIS	L611	L549	R488	C427	I367
I1226	V1165	H1104	R1043	G980	L920	L857	V797	T736	ASP	M612	L550	R489	G428	K368
A1227	G1166	L1105	P1044	A981	Q921	L858	S798	N737	GLN	E614	D551	D490	K429	P369
H1228	D1167	R1106	S1045	N982	I922	A859	S799	G738	ASP	R615	E552	V491	S430	S370
R1229	K1168	A1107	I1046	G985	P923	I860	F800	Q739	ARG	K815	A553	T492	T431	I371
L1230	G1169	Q1108	P1047	Q986	I924	V861	D801	P740	LYS	G616	T554	T493	T432	D372
S1231	T1170	L1109	V1048	R986	R925	P862	D802	P741	LYS	L617	T555	D494	V433	S373
T1232	Q1171	G1110	L1049	V987	N926	I863	F803	E742	SER	Y618	E495	E496	Q434	F374
K1233	L1172	I1111	Q1050	S988	A927	I864	R804	T743	THR	F619	D568	I496	L435	S375
K1234	S1173	V1112	G1051	S989	N928	A865	R805	Q746	LYS	K620	T559	E497	M436	K376
M1235	G1174	S1113	L1052	F990	Q929	I866	T806	Q747	GLU	L621	E560	K498	Q437	S377
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	K1176	E1115	L1054	P992	A931		G808	S748		Q625	E562	V500	L439	R379
I1239	K1177	P1116	E1055	D993	H932	V870	A809	N749		T626	A663	K501	Y440	K380
V1240	Q1178	I1117	V1056	Y994	V933	E871	L810	L750	V688	ALA	V564	E502	D441	P381
V1241	L1118	T1118	K1057	A995	F934	M872	T811	F751	P689	GLY	V565	A503	P442	D382
I1242	F1119	K1058	K996	K997	G935		T812	S752	P690	ASN	Q566	N504	L443	I383
D1243	D1120	Q1059	A997	A997	I936	L875	R813	L753	A691	ASN	A567	A505	D444	I384
M1244	G1121	Q1060	T998	T998	T937		L814	L754	S692	GLU	A568	Y506	G445	Q385
G1245	S1122	T1061	V999	V999	F938	Q878	A815	F755	F693	I1E	L569	D507	M446	G386
K1246	I1123	L1062	S1000	S939	S939	A879	R816	L756	V694	GLU	D570	F508	V447	I387
V1247	A1063	A1063	A1001	F940	T941	L880	D817	I757	R695	LEU	K571	I509	S448	L388
K1248	L1186	E1125	L1064	T941	Q942	K881	A818	L758	L696	GLY	A572	M510	I449	F389
E1249	Y1187	H1126	V1065	H1093	Q942	D882	A819	G759	L697	ASN	R573	K511	D450	F390
H1250	R1188	T1127	G1066	I1004	A943	K883	Q820	I760	R698	GLU	E574	L512	D453	K391
G1251	L1189	A1128	S1067	I1005	I944	K884	R821	I761	L699	ALA	G575	P513	I454	I392
T1252	P1190	Y1129	S1068	R1006	F945	E885	A835	S762	N700	CYS	R576	H514	I455	I393
H1253	H1191	G1130	G1069	I1007	Y946	L886	Q823	F763	S701	LVS	T577	Q515	R455	H394
Q1254	L1192	D1131	G1070	E1008	F947	E887	A824	I764	T702	SER	T578	F516	T456	F395
Q1255	L1193	H1132	G1071	E1009	S943	G888	T825	I765	E703	LVS	I579	D517	I457	S396
L1256	L1194	S1133	K1072	K1010	I949	S889	G826	F766	W704	ASP	V580	T518	M488	S397
L1257	L1195	P1011	T1011	A950	A950	G890	S827	L768	P705	GLU	I581	L519	V459	P398
A1258	V1135	V1135	P1012	E1013	C952	I892	R829	Q769	F707	ASP	H583	G521	R460	S399
Q1259	V1136	S1137	E1014	F953	F953	A893	L830	G770	W708	ASN	R584	E522	L462	R401
K1260	Y1138	Y1138	D1015	R954	R954	T894	V831	F771	V709	LEU	L585	R523	Y461	E402
G1261	S1200	E1139	L1078	F955	F955	E895	I832	T772	G710	ASP	V588	G524	E463	E403
I1262			S1016	G956	G956	A896	F833	F773	T711	MET			E464	Q404
Y1263	T1019	I1142	T1019	A957	A957	I897	Q834	G774	F712	SER	R589	L527	I466	L405
F1264	Q1020	V1142	Q1082	Y958	Y958	E898	R835	K775	C713	SER	N590	S528	G467	L406
M1266	G1021	R1143	Y1083	L959	L959	N899	I836	A714	A714	LVS	A591	G529	V468	K407
V1267	L1022	A1144	D1084	V960	V960	F900	A837	G777	I715	ASP	D592	G530	V469	G408
	K1023	A1145	P1085	T961	T961	R901	R838	E778	I716	SER	V893	Q531	S470	L409
Q1270	P1024	K1146	M1086	Q962	Q962	T902	L839	I779	M717	GLY	I594	K532	Q471	N410
A1271	M1025	E1147	A1087	N963	N963	V903	G840	L780	G718	SER	A595	Q533	E472	L411
ALA	M1026	A1148	G1038	L964	L964	V904	T841	T781	G719	SER	G596	R534	P473	K412
LVS	L1027	S1089	L1027	N965	N965	S905	S842	K782	L720	LEU	F597	I535	V474	V413
ARG	E1028	I1150	E1028	T966	T966	L906	I843	R783	Q721	I1E	D598	A536	I475	K414
	F1091	H1151	F1091	F967	F967	T907	I844	L784	P722	ARG	G599	I537	F476	S415
SER	V1031	Q1152	L1092	E968	E968	R808	I845	R785	A723	ARG	G600	A538	A477	G416
THR	Q1032	F1153	D1093	R969	R969	E909	S846	Y786		ARG	V601	R539	T478	Q417
VAL	F1033	I1154	G1034	V970	V970	Q910	L847	T877	V726	SER	I602	A540	T479	T418
HIS	S1034	D1155	K1095	L971	L971	K911	I848	V788	I727	THR	V603	L541	I480	V419
HIS	G1035	E1096	E1096	L972	L972	F912	X869	F789	F728	ARG	E604	V542	A481	A420
HIS	V1036	L1087	I1087	V973	V973	E913	G850	K790	S729	LVS	Q605	R543	E482	L421
HIS	P1158	P1158	K1098	F974	F974	R914	R851	T914	S791	SER	G606	R544	M483	G422
HIS	Q1099	F1038	S975	S975	S975	M915	Q852	M792	V731	I1E	N607	P545	I484	G423
HIS	N1039	L1100		A976	A976	Y916	L853	L793	V732	CYS	H608	K546	R485	N424

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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(°)	Ideal(°)
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 ⓘ

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 [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](#)

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(°)	Ideal(°)
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 ⓘ

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 [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%)	-0.55	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 [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	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.