



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:38 AM GMT

PDB ID : 2AJL  
Title : X-ray Structure of Novel Biaryl-Based Dipeptidyl peptidase IV inhibitor  
Authors : Qiao, L.; Baumann, C.A.; Crysler, C.S.; Ninan, N.S.; Abad, M.C.; Spurlino, J.C.; DesJarlais, R.L.; Kervinen, J.; Neeper, M.P.; Bayoumy, S.S.  
Deposited on : 2005-08-02  
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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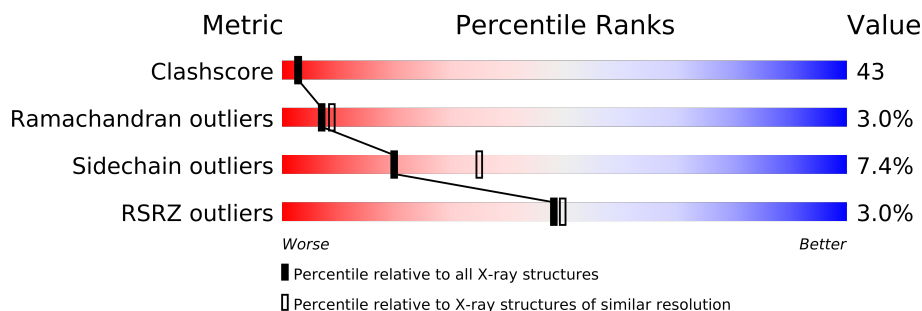
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

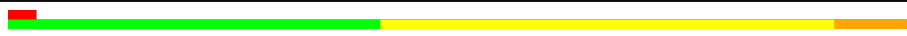
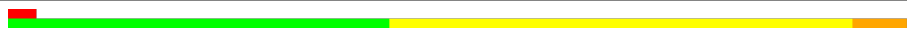
The reported resolution of this entry is 2.50 Å.

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))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	I	728	
1	J	728	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	I	769	-	X
2	NAG	I	770	-	X
2	NAG	J	769	-	X
2	NAG	J	770	-	X
2	NAG	J	771	-	X
2	NAG	J	772	-	X
2	NAG	J	774	-	X
2	NAG	J	775	-	X
3	JNH	I	1	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	JNH	J	1	-	X

## 2 Entry composition i

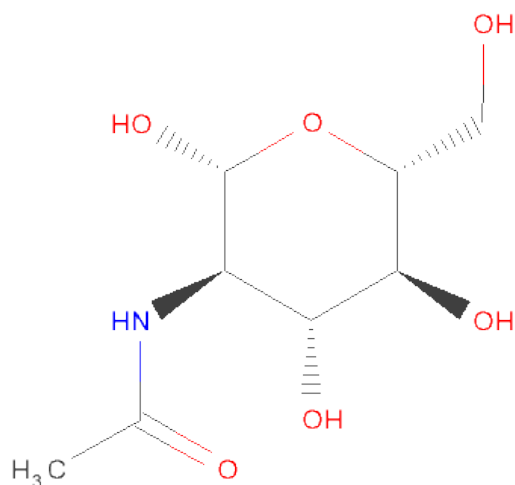
There are 4 unique types of molecules in this entry. The entry contains 12558 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	726	Total	C	N	O	S	0	0	0
			5947	3818	977	1126	26			
1	J	728	Total	C	N	O	S	0	0	0
			5964	3827	982	1129	26			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



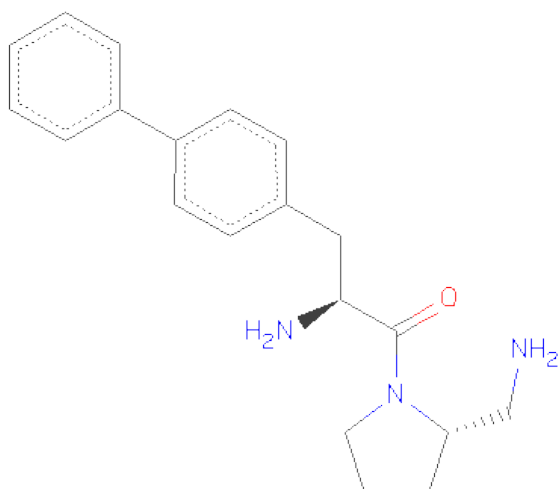
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 1-[2-(S)-AMINO-3-BIPHENYL-4-YL-PROPIONYL]-PYRROLIDINE-2-(S)-CARBONITRILE (three-letter code: JNH) (formula: C<sub>20</sub>H<sub>25</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	1	Total	C	N	O	0	0
			24	20	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	J	1	Total	C	N	O	0	0
			24	20	3	1		

- Molecule 4 is water.

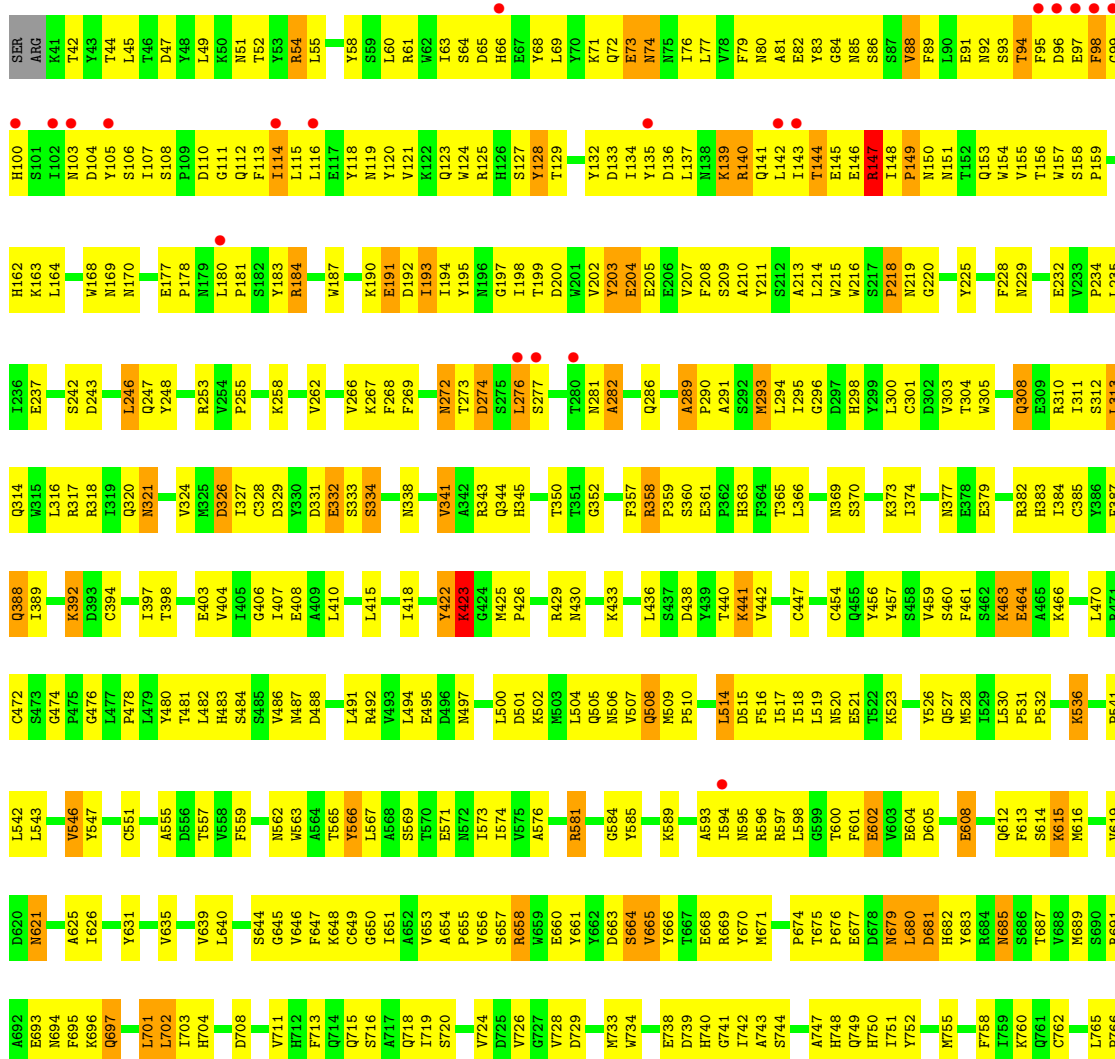
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	190	Total	O	0	0
			190	190		
4	J	213	Total	O	0	0
			213	213		

### 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: Dipeptidyl peptidase 4

Chain I: 



- Molecule 1: Dipeptidyl peptidase 4

Chain J: 

Q718	Q719	S720	K721	V724	D725	V726	G727	C649	G650	I651	P655	M733	M734	S735	T736	D737	E738	D739	H740	G741	I742	H750	I751	M754	M755	I759	K760	F763	S764	L765	P766	Y547	Q553	K554	A555	D556	T557	V558	F559	N562	T565	Y566	L567	A568	S569	T570	E571	E572	I573	A576	S577	F578	D579	Q580	R581	H592	R596	R597	L598	T595	T600	F601	E602	V603	E604	D605	Q606	I607	E608	A609	R611	Q612	F613	S614	K615	M616	G617	F618	V619	D620	N621	K622	R623	L626	M627	Y631	G633	V639	L640	C649	G650	I651	P655	M656	S657	R658	V659	E660	Y661	D662	D663	S664	V665	E666	T667	E668	R669	M670	M671	G672	L673	P674	T675	P676	E677	D678	R679	L680	Y683	T687	V688	M689	S690	E699	Y700	L701	L702	I703	H704	V711	H712	F713	Q714	Q715	P478	L479	Y480	S484	S485	V486	N487	D488	K489	G490	L491	L494	E495	D496	N497	L500	D501	K502	M503	L504	D505	N506	V507	Q508	R509	P510	S511	K512	K513	L514	D515	F516	L517	L518	T522	K523	F524	V525	Y526	O527	M528	L529	L530	E531	P532	H533	F534	D535	Y540	P541	L542	L543	L544	D545	V546	D413	Y414	L415	I418	Y422	K423	G427	G428	R429	M430	L431	Y432	K433	I434	Q435	L436	S437	D438	Y439	T440	K441	Y442	T443	C444	L445	S446	E447	E448	L449	M450	P451	G452	R453	C454	Q455	Y456	Y457	S458	V459	S460	F461	S462	K463	E464	A465	K466	Y467	Y468	Q469	T470	R471	C472	S473	G474	P475	G476	L477	K625	D326	I327	C328	D329	Y330	D331	E332	S333	K334	G335	R336	W337	Q344	I345	I346	F347	K348	R358	D373	P359	S360	E361	Y372	K373	L374	S375	S376	R377	E378	E379	G380	G381	R382	H383	I384	C385	Y386	F387	Q388	F461	S462	K463	E464	A465	K466	Y467	Y468	Q469	T470	R471	C472	S473	G474	P475	G476	L477	K391	K392	L397	T398	K399	G400	T401	L407	E408	K409	L410	T411	S412	L246	Q247	Y248	P249	K250	V254	P255	Y256	K257	P258	E259	V262	T265	V266	K267	F268	V271	N272	T273	D274	S275	L276	S277	S278	V279	T280	N281	Q286	L287	T288	A289	P290	M293	D297	H298	Y299	T221	L300	C301	D302	V303	T304	Q308	E309	R310	L313	Q314	W315	R318	I319	Q320	N321	V167	W168	N169	M170	I171	I172	Y173	V174	K175	E176	E177	P178	M179	L180	P181	S182	Y183	R184	W187	G197	Y203	E204	E205	E206	V207	F208	S209	A210	Y211	S212	D213	A213	L214	W215	K216	S217	P218	N219	I143	T144	E145	T221	F222	L223	Q227	F228	F229	N229	E232	V233	P234	L235	I236	E237	F240	Y241	Q242	N103	D104	Y105	S106	I107	S108	P109	D110	G111	L112	F113	K114	T115	L116	E117	L118	S119	Y120	Q123	W124	R125	H126	S127	Y128	T129	A130	S131	Y132	D133	I134	Y135	D136	L137	N138	K139	R140	Q141	L142	E143	T144	E145	T221	F222	L223	Q227	F228	F229	N229	E232	V233	P234	L235	I236	E237	F240	Y241	Q242	N150	Q153	V154	V155	T156	W157	S158	P159	V160	G161	H162	K163	S389	R340	Y343	L344	T345	D346	N347	S348	K349	L350	T351	D352	E353	F354	K355	L356	T357	S358	P359	V360	E361	F362	G363	H364	I365	J366	K367	L368	M369	N370	O371	P372	Q373	R374	S375	T376	U377	V378	W379	X380	Y381	Z382	A383	B384	C385	D386	E387	F388	G389	H390	I391	J392	K393	L394	M395	N396	O397	P398	Q399	R400	S401	T402	U403	V404	W405	X406	Y407	Z408	A409	B410	C411	D412	E413	F414	G415	H416	I417	J418	K419	L420	M421	N422	O423	P424	Q425	R426	S427	T428	U429	V430	W431	X432	Y433	Z434	A435	B436	C437	D438	E439	F440	G441	H442	I443	J444	K445	L446	M447	N448	O449	P450	Q451	R452	S453	T454	U455	V456	W457	X458	Y459	Z460	A461	B462	C463	D464	E465	F466	G467	H468	I469	J470	K471	L472	M473	N474	O475	P476	Q477	R478	S479	T480	U481	V482	W483	X484	Y485	Z486	A487	B488	C489	D490	E491	F492	G493	H494	I495	J496	K497	L498	M499	N500	O501	P502	Q503	R504	S505	T506	U507	V508	W509	X510	Y511	Z512	A513	B514	C515	D516	E517	F518	G519	H520	I521	J522	K523	L524	M525	N526	O527	P528	Q529	R530	S531	T532	U533	V534	W535	X536	Y537	Z538	A539	B540	C541	D542	E543	F544	G545	H546	I547	J548	K549	L550	M551	N552	O553	P554	Q555	R556	S557	T558	U559	V560	W561	X562	Y563	Z564	A565	B566	C567	D568	E569	F570	G571	H572	I573	J574	K575	L576	M577	N578	O579	P580	Q581	R582	S583	T584	U585	V586	W587	X588	Y589	Z590	A591	B592	C593	D594	E595	F596	G597	H598	I599	J600	K601	L602	M603	N604	O605	P606	Q607	R608	S609	T610	U611	V612	W613	X614	Y615	Z616	A617	B618	C619	D620	E621	F622	G623	H624	I625	J626	K627	L628	M629	N630	O631	P632	Q633	R634	S635	T636	U637	V638	W639	X640	Y641	Z642	A643	B644	C645	D646	E647	F648	G649	H650	I651	J652	K653	L654	M655	N656	O657	P658	Q659	R660	S661	T662	U663	V664	W665	X666	Y667	Z668	A669	B670	C671	D672	E673	F674	G675	H676	I677	J678	K679	L680	M681	N682	O683	P684	Q685	R686	S687	T688	U689	V690	W691	X692	Y693	Z694	A695	B696	C697	D698	E699	F700	G701	H702	I703	J704	K705	L706	M707	N708	O709	P710	Q711	R712	S713	T714	U715	V716	W717	X718	Y719	Z720	A721	B722	C723	D724	E725	F726	G727	H728	I729	J730	K731	L732	M733	N734	O735	P736	Q737	R738	S739	T740	U741	V742	W743	X744	Y745	Z746	A747	B748	C749	D750	E751	F752	G753	H754	I755	J756	K757	L758	M759	N760	O761	P762	Q763	R764	S765	T766	U767	V768	W769	X770	Y771	Z772	A773	B774	C775	D776	E777	F778	G779	H780	I781	J782	K783	L784	M785	N786	O787	P788	Q789	R790	S791	T792	U793	V794	W795	X796	Y797	Z798	A799	B800	C801	D802	E803	F804	G805	H806	I807	J808	K809	L810	M811	N812	O813	P814	Q815	R816	S817	T818	U819	V820	W821	X822	Y823	Z824	A825	B826	C827	D828	E829	F830	G831	H832	I833	J834	K835	L836	M837	N838	O839	P840	Q841	R842	S843	T844	U845	V846	W847	X848	Y849	Z850	A851	B852	C853	D854	E855	F856	G857	H858	I859	J860	K861	L862	M863	N864	O865	P866	Q867	R868	S869	T870	U871	V872	W873	X874	Y875	Z876	A877	B878	C879	D880	E881	F882	G883	H884	I885	J886	K887	L888	M889	N890	O891	P892	Q893	R894	S895	T896	U897	V898	W899	X900	Y901	Z902	A903	B904	C905	D906	E907	F908	G909	H910	I911	J912	K913	L914	M915	N916	O917	P918	Q919	R920	S921	T922	U923	V924	W925	X926	Y927	Z928	A929	B930	C931	D932	E933	F934	G935	H936	I937	J938	K939	L940	M941	N942	O943	P944	Q945	R946	S947	T948	U949	V950	W951	X952	Y953	Z954	A955	B956	C957	D958	E959	F960	G961	H962	I963	J964	K965	L966	M967	N968	O969	P970	Q971	R972	S973	T974	U975	V976	W977	X978	Y979	Z980	A981	B982	C983	D984	E985	F986	G987	H988	I989	J990	K991	L992	M993	N994	O995	P996	Q997	R998	S999	T1000	U1001	V1002	W1003	X1004	Y1005	Z1006	A1007	B1008	C1009	D1010	E1011	F1012	G1013	H1014	I1015	J1016	K1017	L1018	M1019	N1020	O1021	P1022	Q1023	R1024	S1025	T1026	U1027	V1028	W1029	X1030	Y1031	Z1032	A1033	B1034	C1035	D1036	E1037	F1038	G1039	H1040	I1041	J1042	K1043	L1044	M1045	N1046	O1047	P1048	Q1049	R1050	S1051	T1052	U1053	V1054	W1055	X1056	Y1057	Z1058	A1059	B1060	C1061	D1062	E1063	F1064	G1065	H1066	I1067	J1068	K1069	L1070	M1071	N1072	O1073	P1074	Q1075	R1076	S1077	T1078	U1079	V1080	W1081	X1082	Y1083	Z1084	A1085	B1086	C1087	D1088	E1089	F1090	G1091	H1092	I1093	J1094	K1095	L1096	M1097	N1098	O1099	P1100	Q1101	R1102	S1103	T1104	U1105	V1106	W1107	X1108	Y1109	Z1110	A1111	B1112	C1113	D1114	E1115	F1116	G1117	H1118	I1119	J1120	K1121	L1122	M1123	N1124	O1125	P1126	Q1127	R1128	S1129	T1130	U1131	V1132	W1133	X1134	Y1135	Z1136	A1137	B1138	C1139	D1140	E1141	F1142	G1143	H1144	I1145	J1146	K1147	L1148	M1149	N1150	Q1151	R1152	S1153	T1154	U1155	V1156	W1157	X1158	Y1159	Z1160	A1161	B1162	C1163	D1164	E1165	F1166	G1167	H1168	I1169	J1170	K1171	L1172	M1173	N1174	O1175	P1176	Q1177	R1178	S1179	T1180	U1181	V1182	W1183	X1184	Y1185	Z1186	A1187	B1188	C1189	D1190	E1191	F1192	G1193	H1194	I1195	J1196	K1197	L1198	M1199	N1200	O1201	P1202	Q1203	R1204	S1205	T1206	U1207	V1208	W1209	X1210	Y1211	Z1212	A1213	B1214	C1215	D1216	E1217	F1218	G1219	H1220	I1221	J1222	K1223	L1224	M1225	N1226	O1227	P1228	Q1229	R1230	S1231	T1232	U1233	V1234	W1235	X1236	Y1237	Z1238	A1239	B1240	C1241	D1242	E1243	F1244	G1245	H1246	I1247	J1248	K1249	L1250	M1251	N1252	O1253	P1254	Q1255	R1256	S1257	T1258	U1259	V1260	W1261	X1262	Y1263	Z1264	A1265	B1266	C1267	D1268	E1269	F1270	G1271	H1272	I1273	J1274	K1275	L1276	M1277	N1278	O1279	P1280	Q1281	R1282	S1283	T1284	U1285	V1286	W1287	X1288	Y1289	Z1290	A1291	B1292	C1293	D1294	E1295	F1296	G1297	H1298	I1299	J1300	K1301	L1302	M1303	N1304	O1305	P1306	Q1307	R1308	S1309	T1310
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.28Å 126.88Å 110.83Å 90.00° 99.41° 90.00°	Depositor
Resolution (Å)	64.10 – 2.50 64.40 – 2.51	Depositor EDS
% Data completeness (in resolution range)	90.8 (64.10-2.50) 91.6 (64.40-2.51)	Depositor EDS
$R_{merge}$	0.37	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.226 , 0.303 0.245 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 22.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	1 of 55940 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	12558	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: JNH, NAG

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	I	0.36	0/6119	0.68	4/8322 (0.0%)
1	J	0.37	0/6136	0.67	4/8344 (0.0%)
All	All	0.36	0/12255	0.68	8/16666 (0.0%)

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	J	0	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	766	PRO	CA-C-O	9.57	143.17	120.20
1	J	766	PRO	CA-C-O	9.20	142.28	120.20
1	I	388	GLN	N-CA-C	-6.01	94.77	111.00
1	I	300	LEU	N-CA-C	-5.72	95.55	111.00
1	J	240	PHE	N-CA-C	-5.27	96.78	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	700	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	5947	0	5666	532	0
1	J	5964	0	5684	500	0
2	I	70	0	65	8	0
2	J	126	0	117	22	0
3	I	24	0	24	7	0
3	J	24	0	23	7	0
4	I	190	0	0	18	0
4	J	213	0	0	13	0
All	All	12558	0	11579	1029	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 43.

The worst 5 of 1029 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:489:LYS:HE3	1:J:491:LEU:HD21	1.27	1.14
1:I:289:ALA:HB1	1:I:290:PRO:HA	1.28	1.13
1:I:107:ILE:HG13	1:I:114:ILE:HG12	1.23	1.11
1:I:310:ARG:HD3	1:I:329:ASP:OD1	1.51	1.10
1:I:626:ILE:HD13	1:I:639:VAL:HG21	1.34	1.10

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	I	724/728 (100%)	607 (84%)	86 (12%)	31 (4%)	4	4
1	J	726/728 (100%)	632 (87%)	82 (11%)	12 (2%)	14	22
All	All	1450/1456 (100%)	1239 (85%)	168 (12%)	43 (3%)	7	9

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	94	THR
1	I	98	PHE
1	I	99	GLY
1	I	140	ARG
1	I	147	ARG

### 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	I	651/653 (100%)	603 (93%)	48 (7%)	20	35
1	J	653/653 (100%)	605 (93%)	48 (7%)	20	35
All	All	1304/1306 (100%)	1208 (93%)	96 (7%)	20	35

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	685	ASN
1	J	137	LEU
1	J	673	LEU
1	I	689	MET
1	J	45	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	621	ASN
1	I	731	GLN
1	J	562	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	I	679	ASN
1	I	694	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

16 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$
3	JNH	I	1	1	26,26,26	1.85	5 (19%)	35,35,35	1.52	7 (20%)
2	NAG	I	767	-	12,14,15	3.10	3 (25%)	15,19,21	2.18	3 (20%)
2	NAG	I	768	-	12,14,15	2.90	3 (25%)	15,19,21	3.12	3 (20%)
2	NAG	I	769	-	12,14,15	2.75	2 (16%)	15,19,21	2.19	4 (26%)
2	NAG	I	770	-	12,14,15	2.90	2 (16%)	15,19,21	2.96	8 (53%)
2	NAG	I	771	-	12,14,15	2.94	3 (25%)	15,19,21	1.69	3 (20%)
3	JNH	J	1	1	26,26,26	1.73	5 (19%)	35,35,35	2.28	9 (25%)
2	NAG	J	767	-	12,14,15	2.89	3 (25%)	15,19,21	3.06	7 (46%)
2	NAG	J	768	-	12,14,15	2.92	2 (16%)	15,19,21	2.77	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	J	769	-	12,14,15	2.94	2 (16%)	15,19,21	2.91	8 (53%)
2	NAG	J	770	-	12,14,15	3.24	4 (33%)	15,19,21	2.45	8 (53%)
2	NAG	J	771	-	12,14,15	3.18	3 (25%)	15,19,21	4.48	5 (33%)
2	NAG	J	772	-	12,14,15	2.89	2 (16%)	15,19,21	2.95	4 (26%)
2	NAG	J	773	-	12,14,15	3.20	4 (33%)	15,19,21	2.27	5 (33%)
2	NAG	J	774	-	12,14,15	2.94	3 (25%)	15,19,21	3.38	7 (46%)
2	NAG	J	775	-	12,14,15	2.92	3 (25%)	15,19,21	2.29	4 (26%)

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
3	JNH	I	1	1	-	0/18/28/28	0/3/3/3
2	NAG	I	767	-	-	1/6/23/26	0/1/1/1
2	NAG	I	768	-	2/2/5/7	0/6/23/26	0/1/1/1
2	NAG	I	769	-	-	1/6/23/26	0/1/1/1
2	NAG	I	770	-	-	0/6/23/26	0/1/1/1
2	NAG	I	771	-	1/1/5/7	0/6/23/26	0/1/1/1
3	JNH	J	1	1	1/1/4/4	0/18/28/28	0/3/3/3
2	NAG	J	767	-	-	0/6/23/26	0/1/1/1
2	NAG	J	768	-	-	0/6/23/26	0/1/1/1
2	NAG	J	769	-	1/1/5/7	0/6/23/26	1/1/1/1
2	NAG	J	770	-	-	0/6/23/26	0/1/1/1
2	NAG	J	771	-	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	J	772	-	-	0/6/23/26	0/1/1/1
2	NAG	J	773	-	-	0/6/23/26	0/1/1/1
2	NAG	J	774	-	-	0/6/23/26	0/1/1/1
2	NAG	J	775	-	-	1/6/23/26	0/1/1/1

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	771	NAG	O7-C7	9.54	1.44	1.23
2	J	773	NAG	O7-C7	9.53	1.44	1.23
2	J	770	NAG	O7-C7	9.48	1.44	1.23
2	I	767	NAG	O7-C7	9.22	1.43	1.23
2	J	768	NAG	O7-C7	9.21	1.43	1.23

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	771	NAG	C2-N2-C7	-15.64	96.83	123.09
2	I	768	NAG	C2-N2-C7	-10.28	105.83	123.09
2	J	768	NAG	C2-N2-C7	-7.79	110.00	123.09
2	J	772	NAG	C2-N2-C7	-7.67	110.20	123.09
2	J	774	NAG	C3-C2-N2	-7.59	100.21	111.76

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	768	NAG	C5
2	I	768	NAG	C3
2	I	771	NAG	C5
2	J	769	NAG	C4
2	J	771	NAG	C3

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	775	NAG	C8-C7-N2-C2
2	I	767	NAG	O7-C7-N2-C2
2	I	769	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	769	NAG	C1-C2-C3-C4-C5-O5

## 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	I	726/728 (99%)	0.26	20 (2%) 50 53	3, 19, 50, 80	0
1	J	728/728 (100%)	0.24	24 (3%) 44 45	3, 16, 49, 86	0
All	All	1454/1456 (99%)	0.25	44 (3%) 48 50	3, 18, 49, 86	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	99	GLY	8.1
1	J	98	PHE	5.4
1	I	98	PHE	4.6
1	I	95	PHE	4.3
1	J	138	ASN	4.0

### 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<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	J	772	14/15	0.23	118.00	56,60,65,65	0
2	NAG	J	770	14/15	0.36	7.13	56,62,69,70	0
3	JNH	I	1	24/24	0.26	3.54	27,32,38,41	0
2	NAG	I	769	14/15	0.28	3.24	59,61,65,66	0
2	NAG	J	775	14/15	0.20	3.21	48,57,60,64	0
2	NAG	J	769	14/15	0.24	3.10	45,50,53,55	0
3	JNH	J	1	24/24	0.22	3.01	19,24,30,30	0
2	NAG	I	770	14/15	0.28	2.50	77,80,81,82	0
2	NAG	J	774	14/15	0.22	2.40	35,38,41,42	0
2	NAG	J	771	14/15	0.21	2.29	18,21,30,31	0
2	NAG	I	767	14/15	0.21	1.84	38,40,42,43	0
2	NAG	I	768	14/15	0.27	1.82	35,40,42,43	0
2	NAG	J	767	14/15	0.23	-0.09	39,46,49,50	0
2	NAG	J	773	14/15	0.17	-0.88	31,38,41,45	0
2	NAG	J	768	14/15	0.27	-	67,70,72,72	0
2	NAG	I	771	14/15	0.29	-	78,82,86,86	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.