



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:01 PM GMT

PDB ID : 4E0S
Title : Crystal Structure of C5b-6
Authors : Aleshin, A.E.; Stec, B.; DiScipio, R.; Liddington, R.C.
Deposited on : 2012-03-05
Resolution : 4.21 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

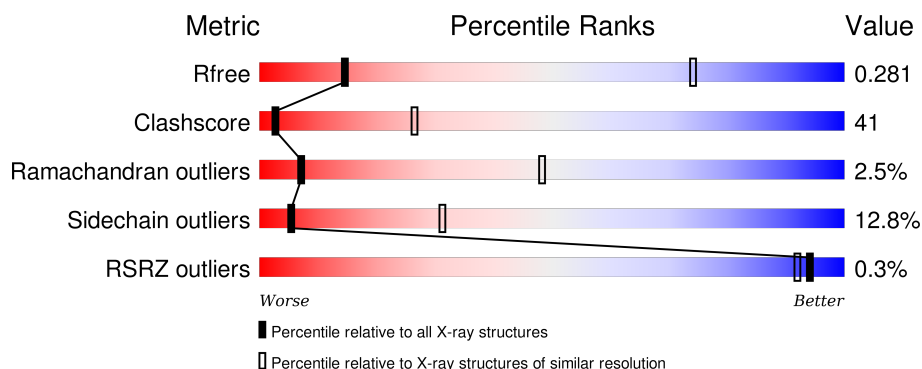
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.21 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	1041 (4.84-3.60)
Clashscore	102246	1143 (4.84-3.60)
Ramachandran outliers	100387	1086 (4.84-3.60)
Sidechain outliers	100360	1070 (4.84-3.60)
RSRZ outliers	91569	1045 (4.84-3.60)

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	1676	
2	B	913	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19475 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1552	Total	C	N	O	S	0	0	0
			12306	7891	2011	2359	45			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	802	ILE	VAL	SEE REMARK 999	UNP P01031

- Molecule 2 is a protein called Complement component C6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	898	Total	C	N	O	S	0	0	0
			7046	4353	1239	1383	71			

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

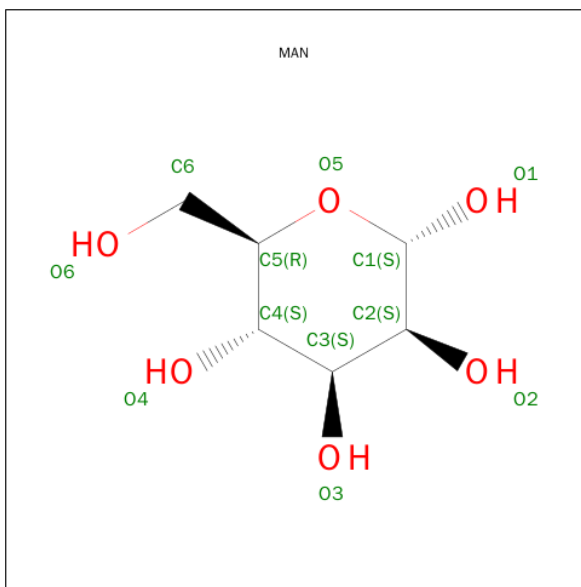
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Ca		0	0
			1	1			

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	2	Total	C	O	0	0
			21	12	9		

- Molecule 7 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).

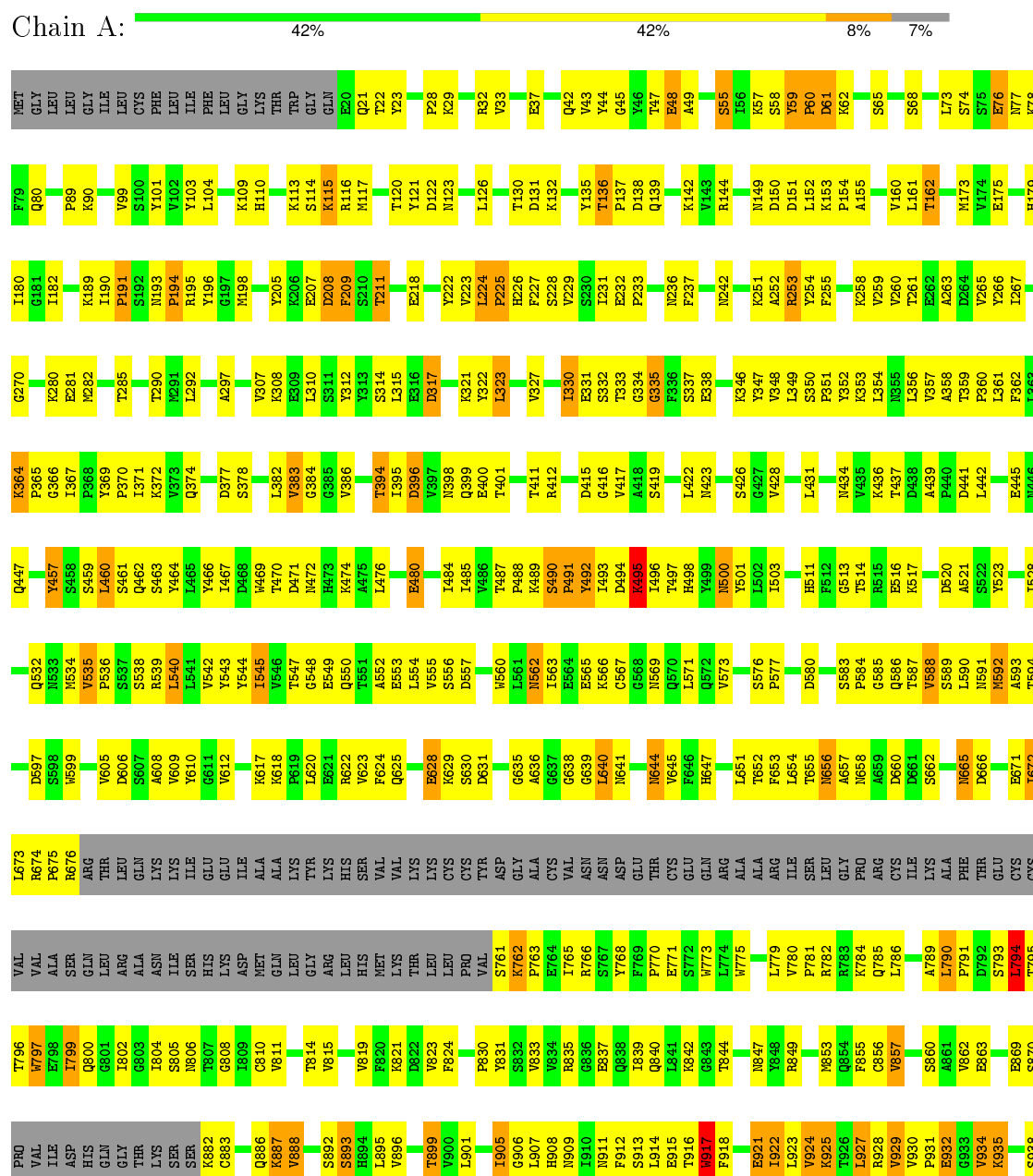


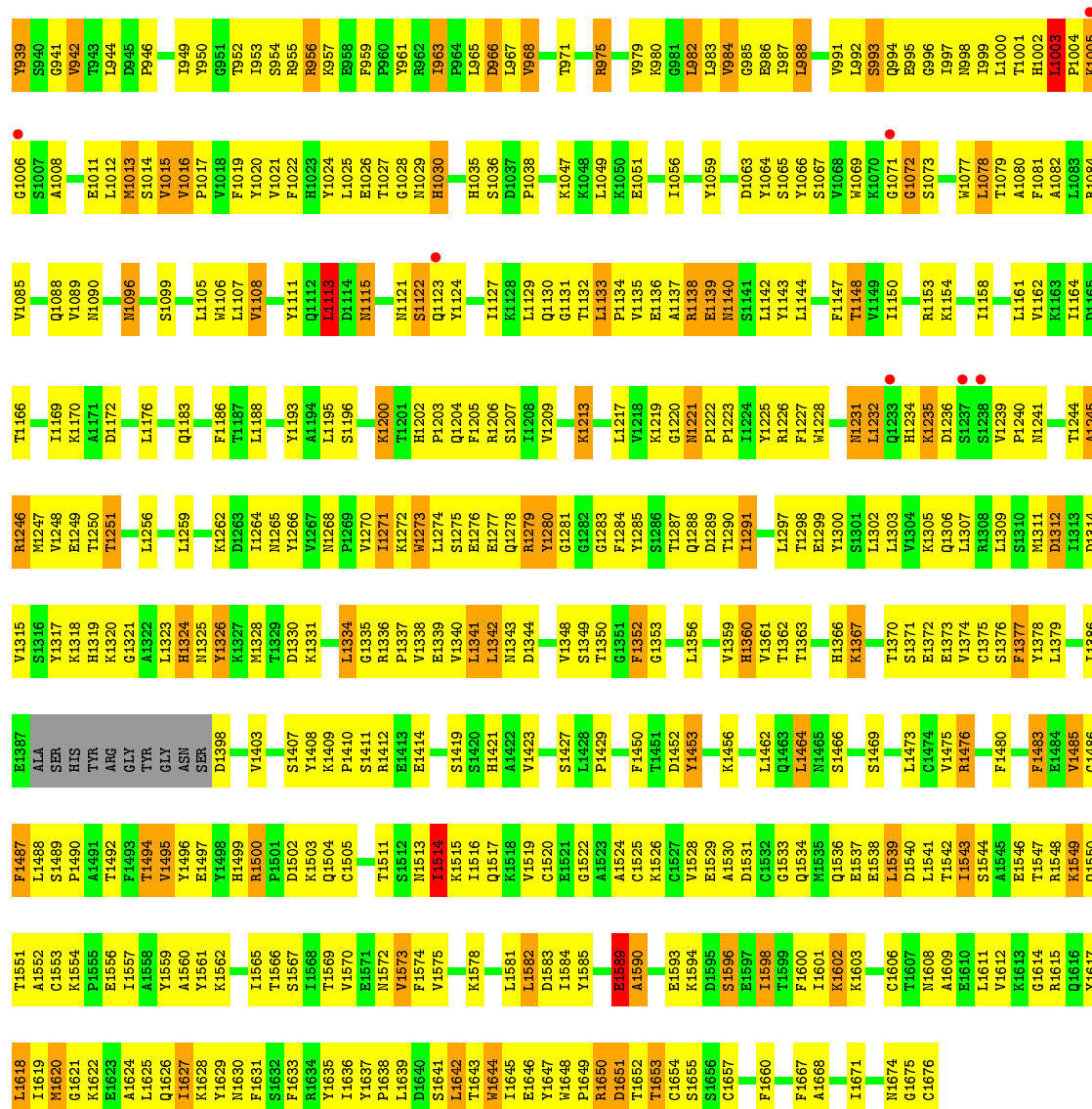
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		

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 ($\text{RSRZ} > 2$). 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.

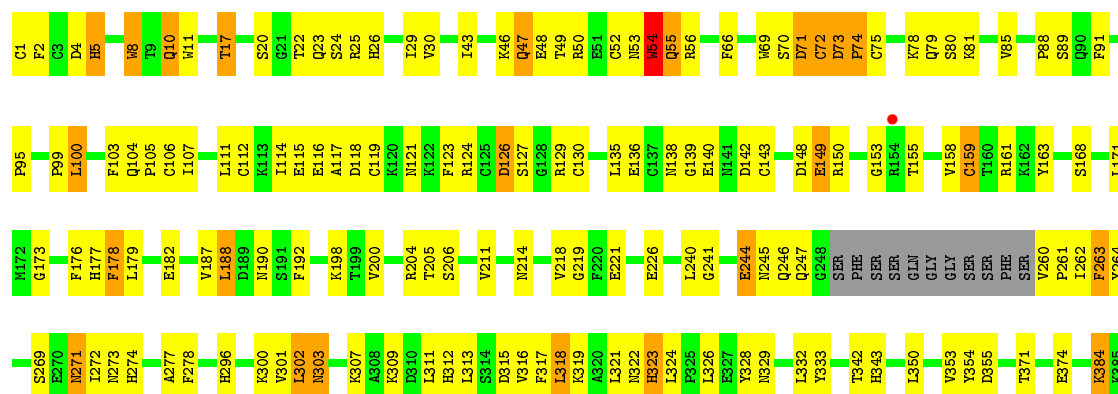
• Molecule 1: Complement C5





• Molecule 2: Complement component C6

Chain B: 54% 37% 7% ..



K482	K483	K484	K485	K489	Y493	A494	A495	K496	F497	D498	P499	Q500	Q501	P506	N507	R508	G509	R510	T516	V521	G528	G442	E529	N530	E444	E445	K446	T447	F448	K451	S454	V455	P459	F464	E465	L466	A467	P468	I469	V470	D471	L472	V473	R474	I475	Y560	K561	P477	C478	A479	V480	T481																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
K486	K487	K488	K489	K490	K491	K492	K493	K494	K495	K496	K497	K498	K499	K500	K501	K502	K503	K504	K505	K506	K507	K508	K509	K510	K511	K512	K513	K514	K515	K516	K517	K518	K519	K520	K521	K522	K523	K524	K525	K526	K527	K528	K529	K530	K531	K532	K533	K534	K535	K536	K537	K538	K539	K540	K541	K542	K543	K544	K545	K546	K547	K548	K549	K550	K551	K552	K553	K554	K555	K556	K557	K558	K559	K560	K561	K562	K563	K564	K565	K566	K567	K568	K569	K570	K571	K572	K573	K574	K575	K576	K577	K578	K579	K580	K581	K582	K583	K584	K585	K586	K587	K588	K589	K590	K591	K592	K593	K594	K595	K596	K597	K598	K599	K600	K601	K602	K603	K604	K605	K606	K607	K608	K609	K610	K611	K612	K613	K614	K615	K616	K617	K618	K619	K620	K621	K622	K623	K624	K625	K626	K627	K628	K629	K630	K631	K632	K633	K634	K635	K636	K637	K638	K639	K640	K641	K642	K643	K644	K645	K646	K647	K648	K649	K650	K651	K652	K653	K654	K655	K656	K657	K658	K659	K660	K661	K662	K663	K664	K665	K666	K667	K668	K669	K670	K671	K672	K673	K674	K675	K676	K677	K678	K679	K680	K681	K682	K683	K684	K685	K686	K687	K688	K689	K690	K691	K692	K693	K694	K695	K696	K697	K698	K699	K700	K701	K702	K703	K704	K705	K706	K707	K708	K709	K710	K711	K712	K713	K714	K715	K716	K717	K718	K719	K720	K721	K722	K723	K724	K725	K726	K727	K728	K729	K730	K731	K732	K733	K734	K735	K736	K737	K738	K739	K740	K741	K742	K743	K744	K745	K746	K747	K748	K749	K750	K751	K752	K753	K754	K755	K756	K757	K758	K759	K760	K761	K762	K763	K764	K765	K766	K767	K768	K769	K770	K771	K772	K773	K774	K775	K776	K777	K778	K779	K780	K781	K782	K783	K784	K785	K786	K787	K788	K789	K790	K791	K792	K793	K794	K795	K796	K797	K798	K799	K800	K801	K802	K803	K804	K805	K806	K807	K808	K809	K810	K811	K812	K813	K814	K815	K816	K817	K818	K819	K820	K821	K822	K823	K824	K825	K826	K827	K828	K829	K830	K831	K832	K833	K834	K835	K836	K837	K838	K839	K840	K841	K842	K843	K844	K845	K846	K847	K848	K849	K850	K851	K852	K853	K854	K855	K856	K857	K858	K859	K860	K861	K862	K863	K864	K865	K866	K867	K868	K869	K870	K871	K872	K873	K874	K875	K876	K877	K878	K879	K880	K881	K882	K883	K884	K885	K886	K887	K888	K889	K890	K891	K892	K893	K894	K895	K896	K897	K898	K899	K900	K901	K902	K903	K904	K905	K906	K907	K908	K909	K910	K911	K912	K913	K914	K915	K916	K917	K918	K919	K920	K921	K922	K923	K924	K925	K926	K927	K928	K929	K930	K931	K932	K933	K934	K935	K936	K937	K938	K939	K940	K941	K942	K943	K944	K945	K946	K947	K948	K949	K950	K951	K952	K953	K954	K955	K956	K957	K958	K959	K960	K961	K962	K963	K964	K965	K966	K967	K968	K969	K970	K971	K972	K973	K974	K975	K976	K977	K978	K979	K980	K981	K982	K983	K984	K985	K986	K987	K988	K989	K990	K991	K992	K993	K994	K995	K996	K997	K998	K999	1000	1001	1002	1003	1004	1005	1006	1007	1008	1009	1010	1011	1012	1013	1014	1015	1016	1017	1018	1019	1020	1021	1022	1023	1024	1025	1026	1027	1028	1029	1030	1031	1032	1033	1034	1035	1036	1037	1038	1039	1040	1041	1042	1043	1044	1045	1046	1047	1048	1049	1050	1051	1052	1053	1054	1055	1056	1057	1058	1059	1060	1061	1062	1063	1064	1065	1066	1067	1068	1069	1070	1071	1072	1073	1074	1075	1076	1077	1078	1079	1080	1081	1082	1083	1084	1085	1086	1087	1088	1089	1090	1091	1092	1093	1094	1095	1096	1097	1098	1099	1100	1101	1102	1103	1104	1105	1106	1107	1108	1109	1110	1111	1112	1113	1114	1115	1116	1117	1118	1119	1120	1121	1122	1123	1124	1125	1126	1127	1128	1129	1130	1131	1132	1133	1134	1135	1136	1137	1138	1139	1140	1141	1142	1143	1144	1145	1146	1147	1148	1149	1150	1151	1152	1153	1154	1155	1156	1157	1158	1159	1160	1161	1162	1163	1164	1165	1166	1167	1168	1169	1170	1171	1172	1173	1174	1175	1176	1177	1178	1179	1180	1181	1182	1183	1184	1185	1186	1187	1188	1189	1190	1191	1192	1193	1194	1195	1196	1197	1198	1199	1200	1201	1202	1203	1204	1205	1206	1207	1208	1209	1210	1211	1212	1213	1214	1215	1216	1217	1218	1219	1220	1221	1222	1223	1224	1225	1226	1227	1228	1229	1230	1231	1232	1233	1234	1235	1236	1237	1238	1239	1240	1241	1242	1243	1244	1245	1246	1247	1248	1249	1250	1251	1252	1253	1254	1255	1256	1257	1258	1259	1260	1261	1262	1263	1264	1265	1266	1267	1268	1269	1270	1271	1272	1273	1274	1275	1276	1277	1278	1279	1280	1281	1282	1283	1284	1285	1286	1287	1288	1289	1290	1291	1292	1293	1294	1295	1296	1297	1298	1299	1300	1301	1302	1303	1304	1305	1306	1307	1308	1309	1310	1311	1312	1313	1314	1315	1316	1317	1318	1319	1320	1321	1322	1323	1324	1325	1326	1327	1328	1329	1330	1331	1332	1333	1334	1335	1336	1337	1338	1339	1340	1341	1342	1343	1344	1345	1346	1347	1348	1349	1350	1351	1352	1353	1354	1355	1356	1357	1358	1359	1360	1361	1362	1363	1364	1365	1366	1367	1368	1369	1370	1371	1372	1373	1374	1375	1376	1377	1378	1379	1380	1381	1382	1383	1384	1385	1386	1387	1388	1389	1390	1391	1392	1393	1394	1395	1396	1397	1398	1399	1400	1401	1402	1403	1404	1405	1406	1407	1408	1409	1410	1411	1412	1413	1414	1415	1416	1417	1418	1419	1420	1421	1422	1423	1424	1425	1426	1427	1428	1429	1430	1431	1432	1433	1434	1435	1436	1437	1438	1439	1440	1441	1442	1443	1444	1445	1446	1447	1448	1449	1450	1451	1452	1453	1454	1455	1456	1457	1458	1459	1460	1461	1462	1463	1464	1465	1466	1467	1468	1469	1470	1471	1472	1473	1474	1475	1476	1477	1478	1479	1480	1481	1482	1483	1484	1485	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4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	158.95Å 227.53Å 278.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 4.21 29.93 – 4.21	Depositor EDS
% Data completeness (in resolution range)	81.8 (29.93-4.21) 82.1 (29.93-4.21)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 4.26Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.218 , 0.278 0.219 , 0.281	Depositor DCC
R_{free} test set	1529 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	113.5	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 124.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 30134 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19475	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: BGC, NAG, NA, CA, FUC, MAN

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	0.58	6/12576 (0.0%)	0.80	4/17068 (0.0%)
2	B	0.58	5/7193 (0.1%)	0.78	5/9708 (0.1%)
All	All	0.58	11/19769 (0.1%)	0.79	9/26776 (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	A	0	2
2	B	0	3
All	All	0	5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	917	TRP	CD2-CE2	5.98	1.48	1.41
1	A	1273	TRP	CD2-CE2	5.97	1.48	1.41
1	A	797	TRP	CD2-CE2	5.75	1.48	1.41
1	A	1077	TRP	CD2-CE2	5.30	1.47	1.41
2	B	436	TRP	CD2-CE2	5.27	1.47	1.41

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	570	ASN	C-N-CD	-8.57	101.73	120.60
2	B	731	THR	C-N-CD	-7.08	105.03	120.60
1	A	794	LEU	CB-CG-CD2	-5.78	101.18	111.00
2	B	627	VAL	CB-CA-C	-5.50	100.96	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	560	TYR	CA-CB-CG	5.41	123.69	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	90	LYS	Peptide
1	A	985	GLY	Peptide
2	B	391	LYS	Peptide
2	B	599	GLY	Peptide
2	B	731	THR	Peptide

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	12306	0	12238	1116	0
2	B	7046	0	6708	482	0
3	A	28	0	25	1	0
3	B	28	0	25	3	0
4	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	21	0	19	0	0
7	B	44	0	40	7	0
All	All	19475	0	19055	1562	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 41.

The worst 5 of 1562 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:A:1598:ILE:HG21	1:A:1637:TYR:CE2	1.45	1.52
1:A:21:GLN:NE2	1:A:45:GLY:HA2	1.32	1.45
1:A:1013:MET:SD	1:A:1129:LEU:HG	1.65	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:ILE:HD12	1:A:1130:GLN:NE2	1.36	1.35
1:A:1539:LEU:HD22	1:A:1540:ASP:N	1.48	1.27

There are no symmetry-related clashes.

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	1544/1676 (92%)	1339 (87%)	170 (11%)	35 (2%)	8	50
2	B	892/913 (98%)	770 (86%)	96 (11%)	26 (3%)	6	45
All	All	2436/2589 (94%)	2109 (87%)	266 (11%)	61 (2%)	7	48

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	PRO
1	A	89	PRO
1	A	191	PRO
1	A	335	GLY
1	A	490	SER

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	1379/1484 (93%)	1183 (86%)	196 (14%)	4	28
2	B	797/810 (98%)	715 (90%)	82 (10%)	9	40
All	All	2176/2294 (95%)	1898 (87%)	278 (13%)	5	31

5 of 278 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1206	ARG
1	A	1453	TYR
2	B	713	LYS
1	A	1232	LEU
1	A	1331	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1231	ASN
1	A	1499	HIS
2	B	636	ASN
1	A	1265	ASN
1	A	1332	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

6 carbohydrates 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	NAG	A	2001	1,3	14,14,15	0.56	0	15,19,21	1.18	2 (13%)
3	NAG	A	2002	3	14,14,15	0.52	0	15,19,21	1.01	0
3	NAG	B	1002	3,2	14,14,15	0.41	0	15,19,21	2.12	1 (6%)
3	NAG	B	1003	3	14,14,15	0.55	0	15,19,21	1.06	2 (13%)
6	FUC	B	1004	2,6	10,10,11	0.64	0	14,14,16	1.70	3 (21%)
6	BGC	B	1005	6	11,11,12	0.71	0	14,15,17	0.91	0

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	NAG	A	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2002	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1002	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	1003	3	-	0/6/23/26	0/1/1/1
6	FUC	B	1004	2,6	-	0/0/17/20	0/1/1/1
6	BGC	B	1005	6	-	0/2/19/22	0/1/1/1

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(°)
3	A	2001	NAG	O4-C4-C3	-2.43	104.86	110.34
3	B	1003	NAG	O4-C4-C3	-2.10	105.62	110.34
3	A	2001	NAG	O7-C7-C8	-2.05	118.31	122.06
6	B	1004	FUC	O5-C5-C4	2.12	113.21	109.53
3	B	1003	NAG	C1-O5-C5	2.39	115.28	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2002	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	NAG	3	0

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
7	MAN	B	1006	2	11,11,12	0.55	0	14,15,17	0.98	1 (7%)
7	MAN	B	1007	2	11,11,12	0.67	0	14,15,17	0.90	0
7	MAN	B	1008	2	11,11,12	0.65	0	14,15,17	1.56	2 (14%)
7	MAN	B	1009	2	11,11,12	0.59	0	14,15,17	1.27	3 (21%)

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
7	MAN	B	1006	2	-	0/2/19/22	0/1/1/1
7	MAN	B	1007	2	-	0/2/19/22	0/1/1/1
7	MAN	B	1008	2	-	0/2/19/22	0/1/1/1
7	MAN	B	1009	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1009	MAN	O5-C1-C2	-2.74	106.41	110.86
7	B	1008	MAN	O5-C1-C2	-2.38	107.00	110.86
7	B	1009	MAN	C1-O5-C5	2.32	115.19	112.25
7	B	1006	MAN	C1-O5-C5	2.34	115.22	112.25
7	B	1009	MAN	C3-C4-C5	2.38	114.34	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1007	MAN	2	0
7	B	1008	MAN	4	0
7	B	1009	MAN	1	0

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	1552/1676 (92%)	-0.62	7 (0%)	91 88	110, 177, 258, 386	0
2	B	898/913 (98%)	-0.53	1 (0%)	95 95	121, 201, 282, 389	0
All	All	2450/2589 (94%)	-0.59	8 (0%)	94 92	110, 187, 269, 389	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1238	SER	5.2
1	A	1006	GLY	2.9
1	A	1237	SER	2.4
1	A	1005	LYS	2.1
2	B	154	ARG	2.1

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](#)

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(Å ²)	Q<0.9
3	NAG	A	2001	14/15	0.93	0.21	0.06	152,160,185,186	0
6	BGC	B	1005	11/12	0.90	0.29	-	187,198,214,224	0
3	NAG	B	1002	14/15	0.81	0.39	-	205,240,279,295	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	B	1003	14/15	0.80	0.53	-	269,286,304,315	0
3	NAG	A	2002	14/15	0.83	0.27	-	207,226,257,262	0
6	FUC	B	1004	10/11	0.97	0.21	-	174,188,192,196	0

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
7	MAN	B	1008	11/12	0.95	0.23	0.54	147,167,176,188	0
7	MAN	B	1009	11/12	0.94	0.25	0.30	178,190,201,215	0
7	MAN	B	1006	11/12	0.88	0.25	0.12	245,260,277,281	0
7	MAN	B	1007	11/12	0.89	0.22	-0.36	205,212,234,240	0
5	CA	B	1001	1/1	0.91	0.06	-2.09	167,167,167,167	1
4	NA	A	2003	1/1	0.81	0.33	-	111,111,111,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.