wwPDB X-ray Structure Validation Summary Report (i)

May 2, 2016 – 07:29 PM EDT

PDB ID	:	5ES4
Title	:	RE-REFINEMENT OF INTEGRIN ALPHAXBETA2 ECTODOMAIN IN THE CLOSED/BENT CONFORMATION
Authors	:	Sen, M.; Springer, T.A.
Deposited on	:	2015-11-16
Resolution	:	3.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

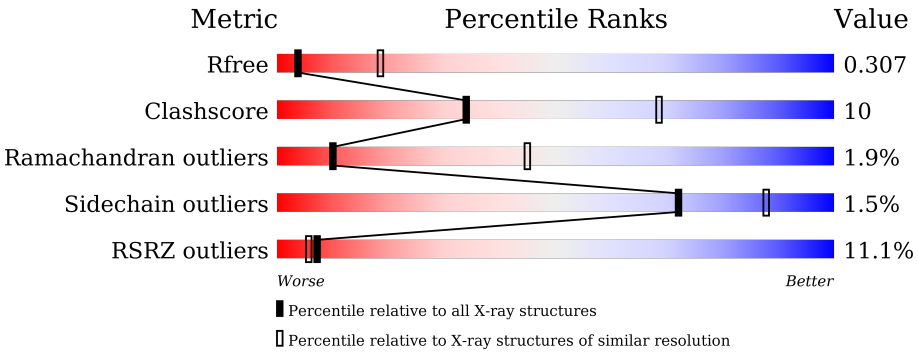
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 <=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	1137	4% 71% 23% • 5%
1	C	1137	9% 58% 19% • 22%
1	E	1137	5% 55% 21% • 22%
1	G	1137	3% 57% 18% • 22%
2	B	727	11% 74% 18% • 7%
2	D	727	27% 71% 20% • 7%

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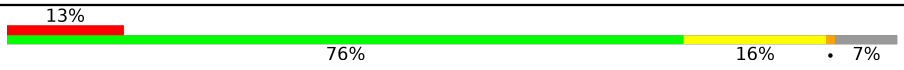
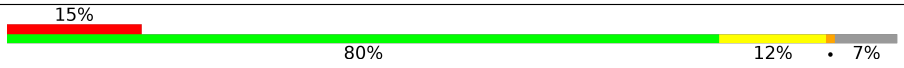
Mol	Chain	Length	Quality of chain
2	F	727	
2	H	727	

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
5	NAG	C	3920	-	-	-	X
5	NAG	D	3232	-	-	-	X
5	NAG	F	3620	-	-	-	X
5	NAG	H	3620	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 51071 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 Integrin alpha-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1080	Total	C	N	O	S	0	0	0
			8371	5289	1451	1593	38			
1	C	884	Total	C	N	O	S	0	3	0
			6834	4314	1188	1298	34			
1	E	884	Total	C	N	O	S	0	3	0
			6838	4317	1187	1300	34			
1	G	883	Total	C	N	O	S	0	1	0
			6787	4287	1170	1296	34			

There are 212 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	GLY	-	expression tag	UNP P20702
A	1086	CYS	-	expression tag	UNP P20702
A	1087	GLY	-	expression tag	UNP P20702
A	1088	GLY	-	expression tag	UNP P20702
A	1089	LEU	-	expression tag	UNP P20702
A	1090	GLU	-	expression tag	UNP P20702
A	1091	ASN	-	expression tag	UNP P20702
A	1092	LEU	-	expression tag	UNP P20702
A	1093	TYR	-	expression tag	UNP P20702
A	1094	PHE	-	expression tag	UNP P20702
A	1095	GLN	-	expression tag	UNP P20702
A	1096	GLY	-	expression tag	UNP P20702
A	1097	GLY	-	expression tag	UNP P20702
A	1098	GLU	-	expression tag	UNP P20702
A	1099	ASN	-	expression tag	UNP P20702
A	1100	ALA	-	expression tag	UNP P20702
A	1101	GLN	-	expression tag	UNP P20702
A	1102	CYS	-	expression tag	UNP P20702
A	1103	GLU	-	expression tag	UNP P20702
A	1104	LYS	-	expression tag	UNP P20702
A	1105	GLU	-	expression tag	UNP P20702

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1106	LEU	-	expression tag	UNP P20702
A	1107	GLN	-	expression tag	UNP P20702
A	1108	ALA	-	expression tag	UNP P20702
A	1109	LEU	-	expression tag	UNP P20702
A	1110	GLU	-	expression tag	UNP P20702
A	1111	LYS	-	expression tag	UNP P20702
A	1112	GLU	-	expression tag	UNP P20702
A	1113	ASN	-	expression tag	UNP P20702
A	1114	ALA	-	expression tag	UNP P20702
A	1115	GLN	-	expression tag	UNP P20702
A	1116	LEU	-	expression tag	UNP P20702
A	1117	GLU	-	expression tag	UNP P20702
A	1118	TRP	-	expression tag	UNP P20702
A	1119	GLU	-	expression tag	UNP P20702
A	1120	LEU	-	expression tag	UNP P20702
A	1121	GLN	-	expression tag	UNP P20702
A	1122	ALA	-	expression tag	UNP P20702
A	1123	LEU	-	expression tag	UNP P20702
A	1124	GLU	-	expression tag	UNP P20702
A	1125	LYS	-	expression tag	UNP P20702
A	1126	GLU	-	expression tag	UNP P20702
A	1127	LEU	-	expression tag	UNP P20702
A	1128	ALA	-	expression tag	UNP P20702
A	1129	GLN	-	expression tag	UNP P20702
A	1130	TRP	-	expression tag	UNP P20702
A	1131	SER	-	expression tag	UNP P20702
A	1132	HIS	-	expression tag	UNP P20702
A	1133	PRO	-	expression tag	UNP P20702
A	1134	GLN	-	expression tag	UNP P20702
A	1135	PHE	-	expression tag	UNP P20702
A	1136	GLU	-	expression tag	UNP P20702
A	1137	LYS	-	expression tag	UNP P20702
C	1085	GLY	-	expression tag	UNP P20702
C	1086	CYS	-	expression tag	UNP P20702
C	1087	GLY	-	expression tag	UNP P20702
C	1088	GLY	-	expression tag	UNP P20702
C	1089	LEU	-	expression tag	UNP P20702
C	1090	GLU	-	expression tag	UNP P20702
C	1091	ASN	-	expression tag	UNP P20702
C	1092	LEU	-	expression tag	UNP P20702
C	1093	TYR	-	expression tag	UNP P20702
C	1094	PHE	-	expression tag	UNP P20702

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1095	GLN	-	expression tag	UNP P20702
C	1096	GLY	-	expression tag	UNP P20702
C	1097	GLY	-	expression tag	UNP P20702
C	1098	GLU	-	expression tag	UNP P20702
C	1099	ASN	-	expression tag	UNP P20702
C	1100	ALA	-	expression tag	UNP P20702
C	1101	GLN	-	expression tag	UNP P20702
C	1102	CYS	-	expression tag	UNP P20702
C	1103	GLU	-	expression tag	UNP P20702
C	1104	LYS	-	expression tag	UNP P20702
C	1105	GLU	-	expression tag	UNP P20702
C	1106	LEU	-	expression tag	UNP P20702
C	1107	GLN	-	expression tag	UNP P20702
C	1108	ALA	-	expression tag	UNP P20702
C	1109	LEU	-	expression tag	UNP P20702
C	1110	GLU	-	expression tag	UNP P20702
C	1111	LYS	-	expression tag	UNP P20702
C	1112	GLU	-	expression tag	UNP P20702
C	1113	ASN	-	expression tag	UNP P20702
C	1114	ALA	-	expression tag	UNP P20702
C	1115	GLN	-	expression tag	UNP P20702
C	1116	LEU	-	expression tag	UNP P20702
C	1117	GLU	-	expression tag	UNP P20702
C	1118	TRP	-	expression tag	UNP P20702
C	1119	GLU	-	expression tag	UNP P20702
C	1120	LEU	-	expression tag	UNP P20702
C	1121	GLN	-	expression tag	UNP P20702
C	1122	ALA	-	expression tag	UNP P20702
C	1123	LEU	-	expression tag	UNP P20702
C	1124	GLU	-	expression tag	UNP P20702
C	1125	LYS	-	expression tag	UNP P20702
C	1126	GLU	-	expression tag	UNP P20702
C	1127	LEU	-	expression tag	UNP P20702
C	1128	ALA	-	expression tag	UNP P20702
C	1129	GLN	-	expression tag	UNP P20702
C	1130	TRP	-	expression tag	UNP P20702
C	1131	SER	-	expression tag	UNP P20702
C	1132	HIS	-	expression tag	UNP P20702
C	1133	PRO	-	expression tag	UNP P20702
C	1134	GLN	-	expression tag	UNP P20702
C	1135	PHE	-	expression tag	UNP P20702
C	1136	GLU	-	expression tag	UNP P20702

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1137	LYS	-	expression tag	UNP P20702
E	1085	GLY	-	expression tag	UNP P20702
E	1086	CYS	-	expression tag	UNP P20702
E	1087	GLY	-	expression tag	UNP P20702
E	1088	GLY	-	expression tag	UNP P20702
E	1089	LEU	-	expression tag	UNP P20702
E	1090	GLU	-	expression tag	UNP P20702
E	1091	ASN	-	expression tag	UNP P20702
E	1092	LEU	-	expression tag	UNP P20702
E	1093	TYR	-	expression tag	UNP P20702
E	1094	PHE	-	expression tag	UNP P20702
E	1095	GLN	-	expression tag	UNP P20702
E	1096	GLY	-	expression tag	UNP P20702
E	1097	GLY	-	expression tag	UNP P20702
E	1098	GLU	-	expression tag	UNP P20702
E	1099	ASN	-	expression tag	UNP P20702
E	1100	ALA	-	expression tag	UNP P20702
E	1101	GLN	-	expression tag	UNP P20702
E	1102	CYS	-	expression tag	UNP P20702
E	1103	GLU	-	expression tag	UNP P20702
E	1104	LYS	-	expression tag	UNP P20702
E	1105	GLU	-	expression tag	UNP P20702
E	1106	LEU	-	expression tag	UNP P20702
E	1107	GLN	-	expression tag	UNP P20702
E	1108	ALA	-	expression tag	UNP P20702
E	1109	LEU	-	expression tag	UNP P20702
E	1110	GLU	-	expression tag	UNP P20702
E	1111	LYS	-	expression tag	UNP P20702
E	1112	GLU	-	expression tag	UNP P20702
E	1113	ASN	-	expression tag	UNP P20702
E	1114	ALA	-	expression tag	UNP P20702
E	1115	GLN	-	expression tag	UNP P20702
E	1116	LEU	-	expression tag	UNP P20702
E	1117	GLU	-	expression tag	UNP P20702
E	1118	TRP	-	expression tag	UNP P20702
E	1119	GLU	-	expression tag	UNP P20702
E	1120	LEU	-	expression tag	UNP P20702
E	1121	GLN	-	expression tag	UNP P20702
E	1122	ALA	-	expression tag	UNP P20702
E	1123	LEU	-	expression tag	UNP P20702
E	1124	GLU	-	expression tag	UNP P20702
E	1125	LYS	-	expression tag	UNP P20702

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1126	GLU	-	expression tag	UNP P20702
E	1127	LEU	-	expression tag	UNP P20702
E	1128	ALA	-	expression tag	UNP P20702
E	1129	GLN	-	expression tag	UNP P20702
E	1130	TRP	-	expression tag	UNP P20702
E	1131	SER	-	expression tag	UNP P20702
E	1132	HIS	-	expression tag	UNP P20702
E	1133	PRO	-	expression tag	UNP P20702
E	1134	GLN	-	expression tag	UNP P20702
E	1135	PHE	-	expression tag	UNP P20702
E	1136	GLU	-	expression tag	UNP P20702
E	1137	LYS	-	expression tag	UNP P20702
G	1085	GLY	-	expression tag	UNP P20702
G	1086	CYS	-	expression tag	UNP P20702
G	1087	GLY	-	expression tag	UNP P20702
G	1088	GLY	-	expression tag	UNP P20702
G	1089	LEU	-	expression tag	UNP P20702
G	1090	GLU	-	expression tag	UNP P20702
G	1091	ASN	-	expression tag	UNP P20702
G	1092	LEU	-	expression tag	UNP P20702
G	1093	TYR	-	expression tag	UNP P20702
G	1094	PHE	-	expression tag	UNP P20702
G	1095	GLN	-	expression tag	UNP P20702
G	1096	GLY	-	expression tag	UNP P20702
G	1097	GLY	-	expression tag	UNP P20702
G	1098	GLU	-	expression tag	UNP P20702
G	1099	ASN	-	expression tag	UNP P20702
G	1100	ALA	-	expression tag	UNP P20702
G	1101	GLN	-	expression tag	UNP P20702
G	1102	CYS	-	expression tag	UNP P20702
G	1103	GLU	-	expression tag	UNP P20702
G	1104	LYS	-	expression tag	UNP P20702
G	1105	GLU	-	expression tag	UNP P20702
G	1106	LEU	-	expression tag	UNP P20702
G	1107	GLN	-	expression tag	UNP P20702
G	1108	ALA	-	expression tag	UNP P20702
G	1109	LEU	-	expression tag	UNP P20702
G	1110	GLU	-	expression tag	UNP P20702
G	1111	LYS	-	expression tag	UNP P20702
G	1112	GLU	-	expression tag	UNP P20702
G	1113	ASN	-	expression tag	UNP P20702
G	1114	ALA	-	expression tag	UNP P20702

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1115	GLN	-	expression tag	UNP P20702
G	1116	LEU	-	expression tag	UNP P20702
G	1117	GLU	-	expression tag	UNP P20702
G	1118	TRP	-	expression tag	UNP P20702
G	1119	GLU	-	expression tag	UNP P20702
G	1120	LEU	-	expression tag	UNP P20702
G	1121	GLN	-	expression tag	UNP P20702
G	1122	ALA	-	expression tag	UNP P20702
G	1123	LEU	-	expression tag	UNP P20702
G	1124	GLU	-	expression tag	UNP P20702
G	1125	LYS	-	expression tag	UNP P20702
G	1126	GLU	-	expression tag	UNP P20702
G	1127	LEU	-	expression tag	UNP P20702
G	1128	ALA	-	expression tag	UNP P20702
G	1129	GLN	-	expression tag	UNP P20702
G	1130	TRP	-	expression tag	UNP P20702
G	1131	SER	-	expression tag	UNP P20702
G	1132	HIS	-	expression tag	UNP P20702
G	1133	PRO	-	expression tag	UNP P20702
G	1134	GLN	-	expression tag	UNP P20702
G	1135	PHE	-	expression tag	UNP P20702
G	1136	GLU	-	expression tag	UNP P20702
G	1137	LYS	-	expression tag	UNP P20702

- Molecule 2 is a protein called Integrin beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	674	Total	C	N	O	S	0	1	0
			5191	3191	932	1004	64			
2	D	674	Total	C	N	O	S	0	0	0
			5178	3183	927	1004	64			
2	F	674	Total	C	N	O	S	0	1	0
			5189	3189	930	1006	64			
2	H	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			

There are 212 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	675	ASP	-	expression tag	UNP P05107
B	676	GLY	-	expression tag	UNP P05107
B	677	CYS	-	expression tag	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
B	678	GLY	-	expression tag	UNP P05107
B	679	LEU	-	expression tag	UNP P05107
B	680	GLU	-	expression tag	UNP P05107
B	681	ASN	-	expression tag	UNP P05107
B	682	LEU	-	expression tag	UNP P05107
B	683	TYR	-	expression tag	UNP P05107
B	684	PHE	-	expression tag	UNP P05107
B	685	GLN	-	expression tag	UNP P05107
B	686	GLY	-	expression tag	UNP P05107
B	687	GLY	-	expression tag	UNP P05107
B	688	LYS	-	expression tag	UNP P05107
B	689	ASN	-	expression tag	UNP P05107
B	690	ALA	-	expression tag	UNP P05107
B	691	GLN	-	expression tag	UNP P05107
B	692	CYS	-	expression tag	UNP P05107
B	693	LYS	-	expression tag	UNP P05107
B	694	LYS	-	expression tag	UNP P05107
B	695	LYS	-	expression tag	UNP P05107
B	696	LEU	-	expression tag	UNP P05107
B	697	GLN	-	expression tag	UNP P05107
B	698	ALA	-	expression tag	UNP P05107
B	699	LEU	-	expression tag	UNP P05107
B	700	LYS	-	expression tag	UNP P05107
B	701	LYS	-	expression tag	UNP P05107
B	702	LYS	-	expression tag	UNP P05107
B	703	ASN	-	expression tag	UNP P05107
B	704	ALA	-	expression tag	UNP P05107
B	705	GLN	-	expression tag	UNP P05107
B	706	LEU	-	expression tag	UNP P05107
B	707	LYS	-	expression tag	UNP P05107
B	708	TRP	-	expression tag	UNP P05107
B	709	LYS	-	expression tag	UNP P05107
B	710	LEU	-	expression tag	UNP P05107
B	711	GLN	-	expression tag	UNP P05107
B	712	ALA	-	expression tag	UNP P05107
B	713	LEU	-	expression tag	UNP P05107
B	714	LYS	-	expression tag	UNP P05107
B	715	LYS	-	expression tag	UNP P05107
B	716	LYS	-	expression tag	UNP P05107
B	717	LEU	-	expression tag	UNP P05107
B	718	ALA	-	expression tag	UNP P05107
B	719	GLN	-	expression tag	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
B	720	GLY	-	expression tag	UNP P05107
B	721	GLY	-	expression tag	UNP P05107
B	722	HIS	-	expression tag	UNP P05107
B	723	HIS	-	expression tag	UNP P05107
B	724	HIS	-	expression tag	UNP P05107
B	725	HIS	-	expression tag	UNP P05107
B	726	HIS	-	expression tag	UNP P05107
B	727	HIS	-	expression tag	UNP P05107
D	675	ASP	-	expression tag	UNP P05107
D	676	GLY	-	expression tag	UNP P05107
D	677	CYS	-	expression tag	UNP P05107
D	678	GLY	-	expression tag	UNP P05107
D	679	LEU	-	expression tag	UNP P05107
D	680	GLU	-	expression tag	UNP P05107
D	681	ASN	-	expression tag	UNP P05107
D	682	LEU	-	expression tag	UNP P05107
D	683	TYR	-	expression tag	UNP P05107
D	684	PHE	-	expression tag	UNP P05107
D	685	GLN	-	expression tag	UNP P05107
D	686	GLY	-	expression tag	UNP P05107
D	687	GLY	-	expression tag	UNP P05107
D	688	LYS	-	expression tag	UNP P05107
D	689	ASN	-	expression tag	UNP P05107
D	690	ALA	-	expression tag	UNP P05107
D	691	GLN	-	expression tag	UNP P05107
D	692	CYS	-	expression tag	UNP P05107
D	693	LYS	-	expression tag	UNP P05107
D	694	LYS	-	expression tag	UNP P05107
D	695	LYS	-	expression tag	UNP P05107
D	696	LEU	-	expression tag	UNP P05107
D	697	GLN	-	expression tag	UNP P05107
D	698	ALA	-	expression tag	UNP P05107
D	699	LEU	-	expression tag	UNP P05107
D	700	LYS	-	expression tag	UNP P05107
D	701	LYS	-	expression tag	UNP P05107
D	702	LYS	-	expression tag	UNP P05107
D	703	ASN	-	expression tag	UNP P05107
D	704	ALA	-	expression tag	UNP P05107
D	705	GLN	-	expression tag	UNP P05107
D	706	LEU	-	expression tag	UNP P05107
D	707	LYS	-	expression tag	UNP P05107
D	708	TRP	-	expression tag	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
D	709	LYS	-	expression tag	UNP P05107
D	710	LEU	-	expression tag	UNP P05107
D	711	GLN	-	expression tag	UNP P05107
D	712	ALA	-	expression tag	UNP P05107
D	713	LEU	-	expression tag	UNP P05107
D	714	LYS	-	expression tag	UNP P05107
D	715	LYS	-	expression tag	UNP P05107
D	716	LYS	-	expression tag	UNP P05107
D	717	LEU	-	expression tag	UNP P05107
D	718	ALA	-	expression tag	UNP P05107
D	719	GLN	-	expression tag	UNP P05107
D	720	GLY	-	expression tag	UNP P05107
D	721	GLY	-	expression tag	UNP P05107
D	722	HIS	-	expression tag	UNP P05107
D	723	HIS	-	expression tag	UNP P05107
D	724	HIS	-	expression tag	UNP P05107
D	725	HIS	-	expression tag	UNP P05107
D	726	HIS	-	expression tag	UNP P05107
D	727	HIS	-	expression tag	UNP P05107
F	675	ASP	-	expression tag	UNP P05107
F	676	GLY	-	expression tag	UNP P05107
F	677	CYS	-	expression tag	UNP P05107
F	678	GLY	-	expression tag	UNP P05107
F	679	LEU	-	expression tag	UNP P05107
F	680	GLU	-	expression tag	UNP P05107
F	681	ASN	-	expression tag	UNP P05107
F	682	LEU	-	expression tag	UNP P05107
F	683	TYR	-	expression tag	UNP P05107
F	684	PHE	-	expression tag	UNP P05107
F	685	GLN	-	expression tag	UNP P05107
F	686	GLY	-	expression tag	UNP P05107
F	687	GLY	-	expression tag	UNP P05107
F	688	LYS	-	expression tag	UNP P05107
F	689	ASN	-	expression tag	UNP P05107
F	690	ALA	-	expression tag	UNP P05107
F	691	GLN	-	expression tag	UNP P05107
F	692	CYS	-	expression tag	UNP P05107
F	693	LYS	-	expression tag	UNP P05107
F	694	LYS	-	expression tag	UNP P05107
F	695	LYS	-	expression tag	UNP P05107
F	696	LEU	-	expression tag	UNP P05107
F	697	GLN	-	expression tag	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
F	698	ALA	-	expression tag	UNP P05107
F	699	LEU	-	expression tag	UNP P05107
F	700	LYS	-	expression tag	UNP P05107
F	701	LYS	-	expression tag	UNP P05107
F	702	LYS	-	expression tag	UNP P05107
F	703	ASN	-	expression tag	UNP P05107
F	704	ALA	-	expression tag	UNP P05107
F	705	GLN	-	expression tag	UNP P05107
F	706	LEU	-	expression tag	UNP P05107
F	707	LYS	-	expression tag	UNP P05107
F	708	TRP	-	expression tag	UNP P05107
F	709	LYS	-	expression tag	UNP P05107
F	710	LEU	-	expression tag	UNP P05107
F	711	GLN	-	expression tag	UNP P05107
F	712	ALA	-	expression tag	UNP P05107
F	713	LEU	-	expression tag	UNP P05107
F	714	LYS	-	expression tag	UNP P05107
F	715	LYS	-	expression tag	UNP P05107
F	716	LYS	-	expression tag	UNP P05107
F	717	LEU	-	expression tag	UNP P05107
F	718	ALA	-	expression tag	UNP P05107
F	719	GLN	-	expression tag	UNP P05107
F	720	GLY	-	expression tag	UNP P05107
F	721	GLY	-	expression tag	UNP P05107
F	722	HIS	-	expression tag	UNP P05107
F	723	HIS	-	expression tag	UNP P05107
F	724	HIS	-	expression tag	UNP P05107
F	725	HIS	-	expression tag	UNP P05107
F	726	HIS	-	expression tag	UNP P05107
F	727	HIS	-	expression tag	UNP P05107
H	675	ASP	-	expression tag	UNP P05107
H	676	GLY	-	expression tag	UNP P05107
H	677	CYS	-	expression tag	UNP P05107
H	678	GLY	-	expression tag	UNP P05107
H	679	LEU	-	expression tag	UNP P05107
H	680	GLU	-	expression tag	UNP P05107
H	681	ASN	-	expression tag	UNP P05107
H	682	LEU	-	expression tag	UNP P05107
H	683	TYR	-	expression tag	UNP P05107
H	684	PHE	-	expression tag	UNP P05107
H	685	GLN	-	expression tag	UNP P05107
H	686	GLY	-	expression tag	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
H	687	GLY	-	expression tag	UNP P05107
H	688	LYS	-	expression tag	UNP P05107
H	689	ASN	-	expression tag	UNP P05107
H	690	ALA	-	expression tag	UNP P05107
H	691	GLN	-	expression tag	UNP P05107
H	692	CYS	-	expression tag	UNP P05107
H	693	LYS	-	expression tag	UNP P05107
H	694	LYS	-	expression tag	UNP P05107
H	695	LYS	-	expression tag	UNP P05107
H	696	LEU	-	expression tag	UNP P05107
H	697	GLN	-	expression tag	UNP P05107
H	698	ALA	-	expression tag	UNP P05107
H	699	LEU	-	expression tag	UNP P05107
H	700	LYS	-	expression tag	UNP P05107
H	701	LYS	-	expression tag	UNP P05107
H	702	LYS	-	expression tag	UNP P05107
H	703	ASN	-	expression tag	UNP P05107
H	704	ALA	-	expression tag	UNP P05107
H	705	GLN	-	expression tag	UNP P05107
H	706	LEU	-	expression tag	UNP P05107
H	707	LYS	-	expression tag	UNP P05107
H	708	TRP	-	expression tag	UNP P05107
H	709	LYS	-	expression tag	UNP P05107
H	710	LEU	-	expression tag	UNP P05107
H	711	GLN	-	expression tag	UNP P05107
H	712	ALA	-	expression tag	UNP P05107
H	713	LEU	-	expression tag	UNP P05107
H	714	LYS	-	expression tag	UNP P05107
H	715	LYS	-	expression tag	UNP P05107
H	716	LYS	-	expression tag	UNP P05107
H	717	LEU	-	expression tag	UNP P05107
H	718	ALA	-	expression tag	UNP P05107
H	719	GLN	-	expression tag	UNP P05107
H	720	GLY	-	expression tag	UNP P05107
H	721	GLY	-	expression tag	UNP P05107
H	722	HIS	-	expression tag	UNP P05107
H	723	HIS	-	expression tag	UNP P05107
H	724	HIS	-	expression tag	UNP P05107
H	725	HIS	-	expression tag	UNP P05107
H	726	HIS	-	expression tag	UNP P05107
H	727	HIS	-	expression tag	UNP P05107

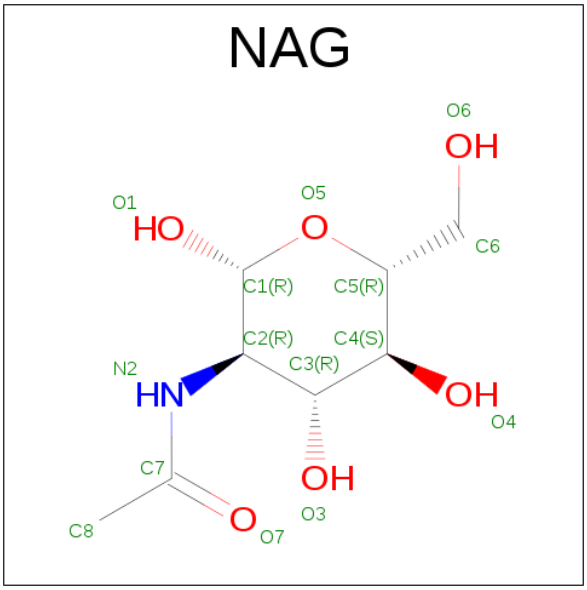
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	3	Total Ca 3 3	0	0
3	D	1	Total Ca 1 1	0	0
3	E	3	Total Ca 3 3	0	0
3	H	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	3	Total Ca 3 3	0	0
3	A	3	Total Ca 3 3	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

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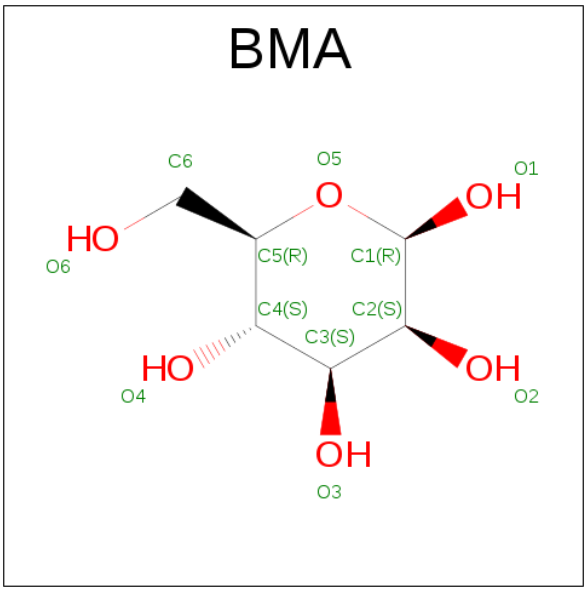
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	C	1	Total C O 11 6 5	0	0
6	C	1	Total C O 11 6 5	0	0
6	C	1	Total C O 11 6 5	0	0
6	C	1	Total C O 11 6 5	0	0
6	E	1	Total C O 11 6 5	0	0
6	E	1	Total C O 11 6 5	0	0
6	E	1	Total C O 11 6 5	0	0
6	E	1	Total C O 11 6 5	0	0
6	G	1	Total C O 11 6 5	0	0
6	G	1	Total C O 11 6 5	0	0

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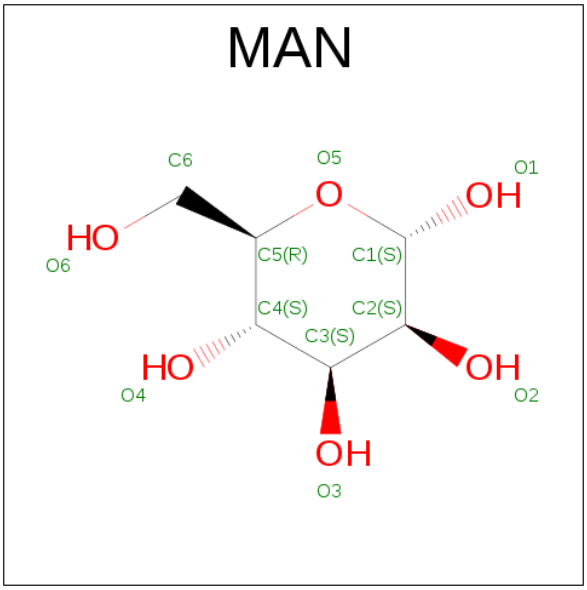
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C O 11 6 5	0	0
6	G	1	Total C O 11 6 5	0	0

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 11 6 5	0	0
7	C	1	Total C O 11 6 5	0	0
7	C	1	Total C O 11 6 5	0	0
7	C	1	Total C O 11 6 5	0	0
7	C	1	Total C O 11 6 5	0	0
7	C	1	Total C O 11 6 5	0	0
7	C	1	Total C O 11 6 5	0	0
7	C	1	Total C O 11 6 5	0	0
7	C	1	Total C O 11 6 5	0	0
7	C	1	Total C O 11 6 5	0	0
7	E	1	Total C O 11 6 5	0	0
7	E	1	Total C O 11 6 5	0	0
7	E	1	Total C O 11 6 5	0	0
7	E	1	Total C O 11 6 5	0	0
7	E	1	Total C O 11 6 5	0	0
7	E	1	Total C O 11 6 5	0	0
7	G	1	Total C O 11 6 5	0	0
7	G	1	Total C O 11 6 5	0	0
7	G	1	Total C O 11 6 5	0	0
7	G	1	Total C O 11 6 5	0	0

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

- Molecule 8 is water.

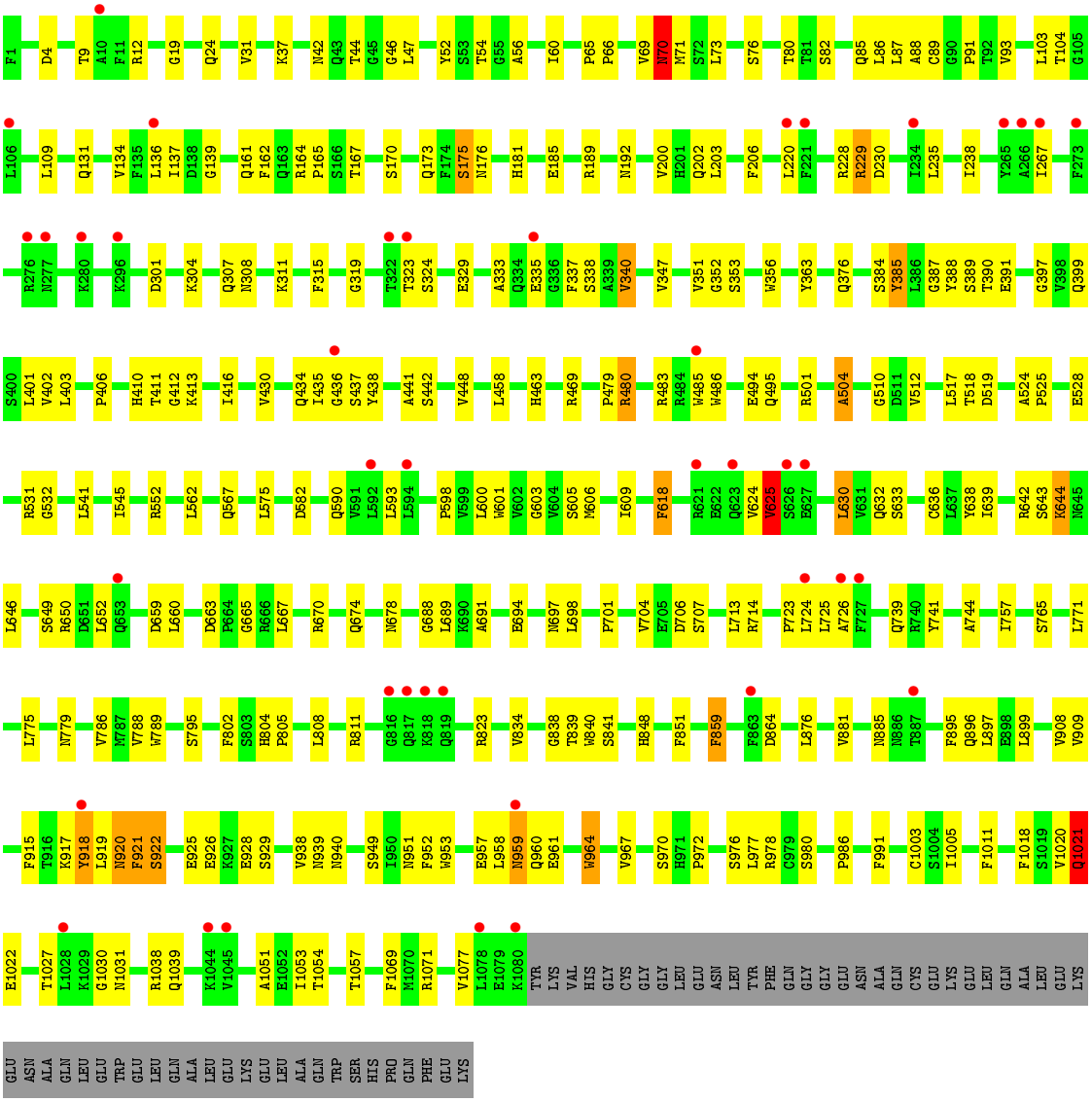
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	29	Total O 29 29	0	0
8	B	4	Total O 4 4	0	0
8	C	7	Total O 7 7	0	0
8	D	3	Total O 3 3	0	0
8	E	10	Total O 10 10	0	0
8	F	2	Total O 2 2	0	0
8	G	10	Total O 10 10	0	0
8	H	2	Total O 2 2	0	0

3 Residue-property plots (i)

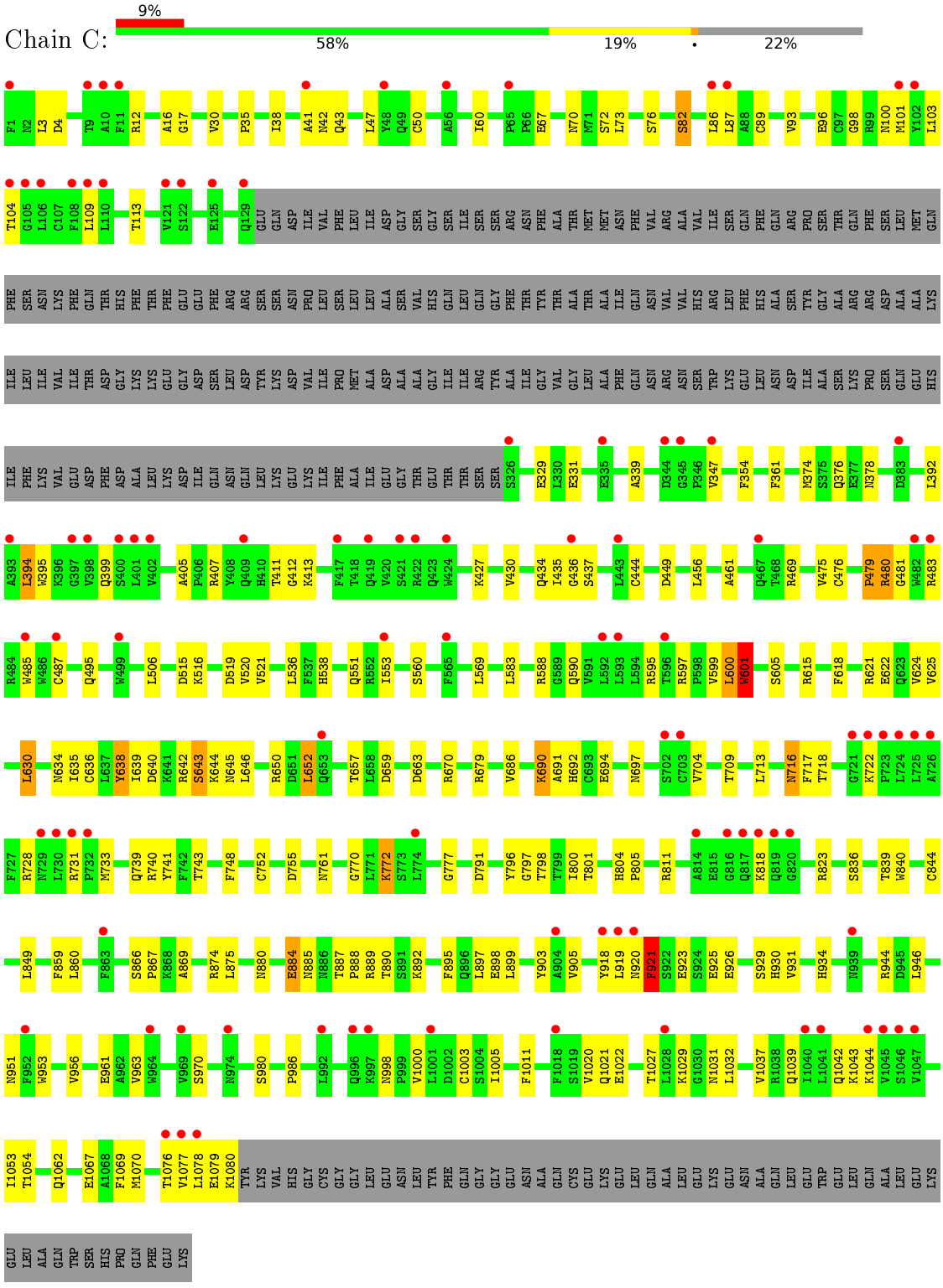
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

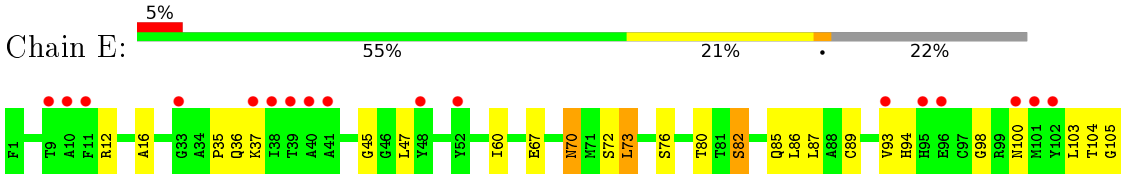
Chain A:

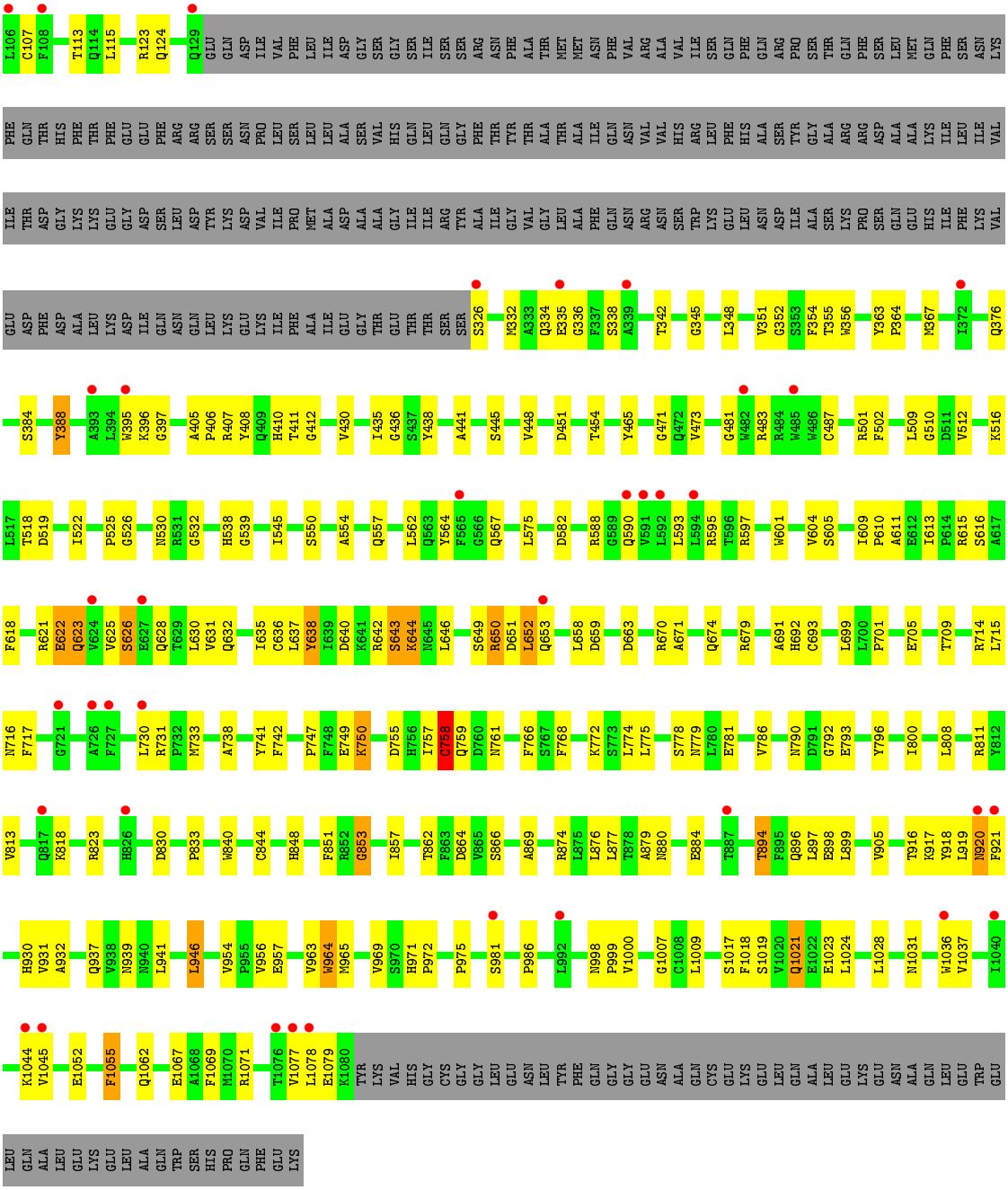


- Molecule 1: Integrin alpha-X



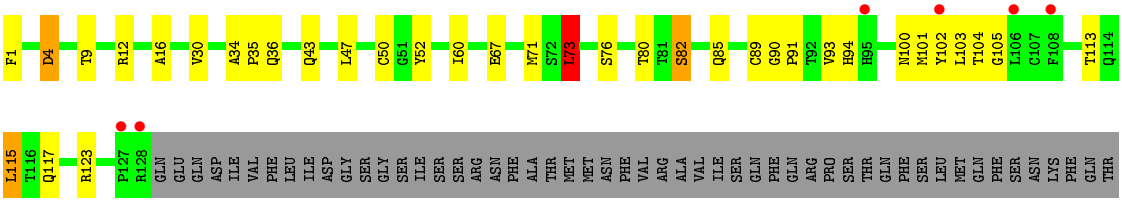
• Molecule 1: Integrin alpha-X

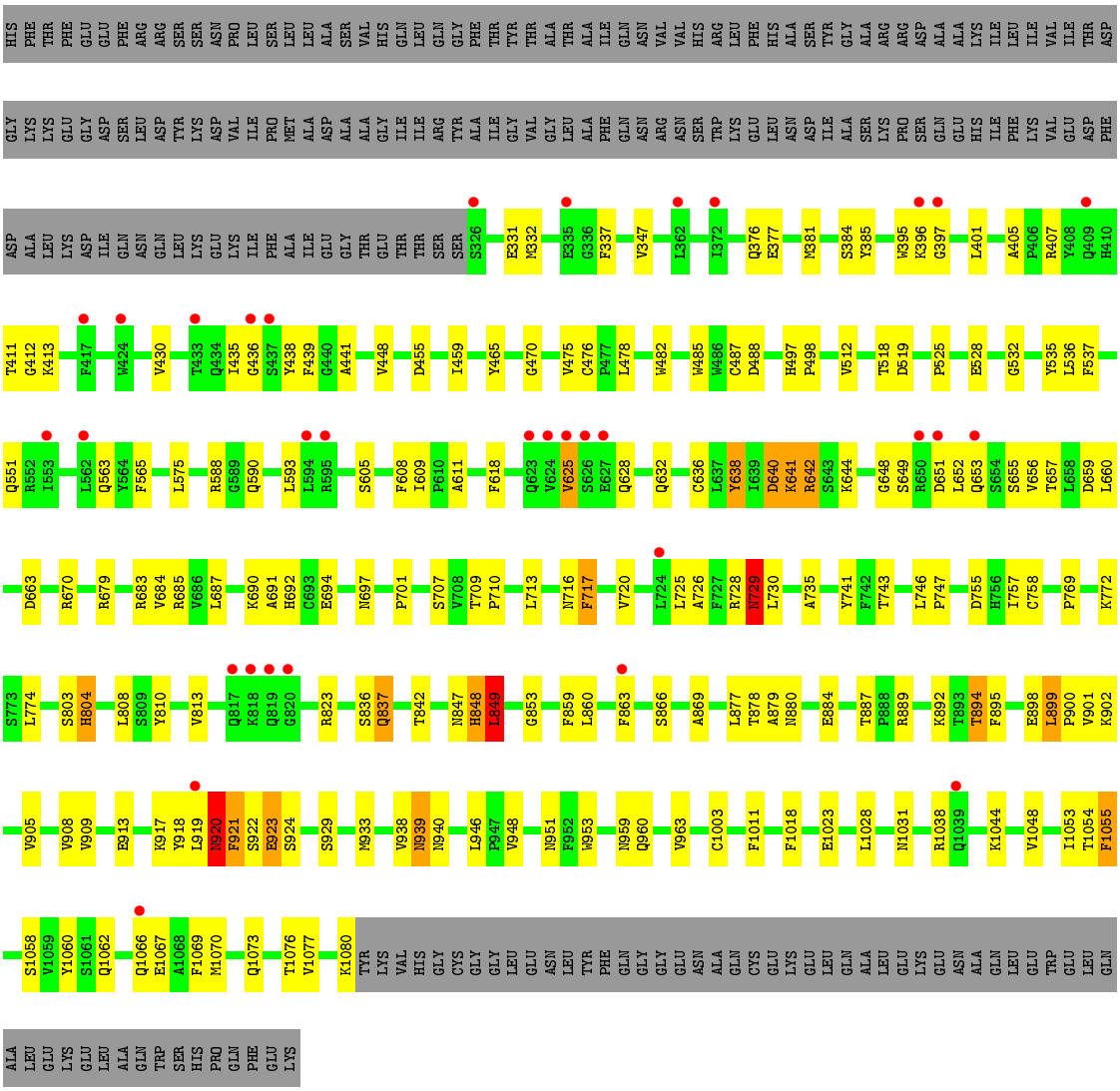




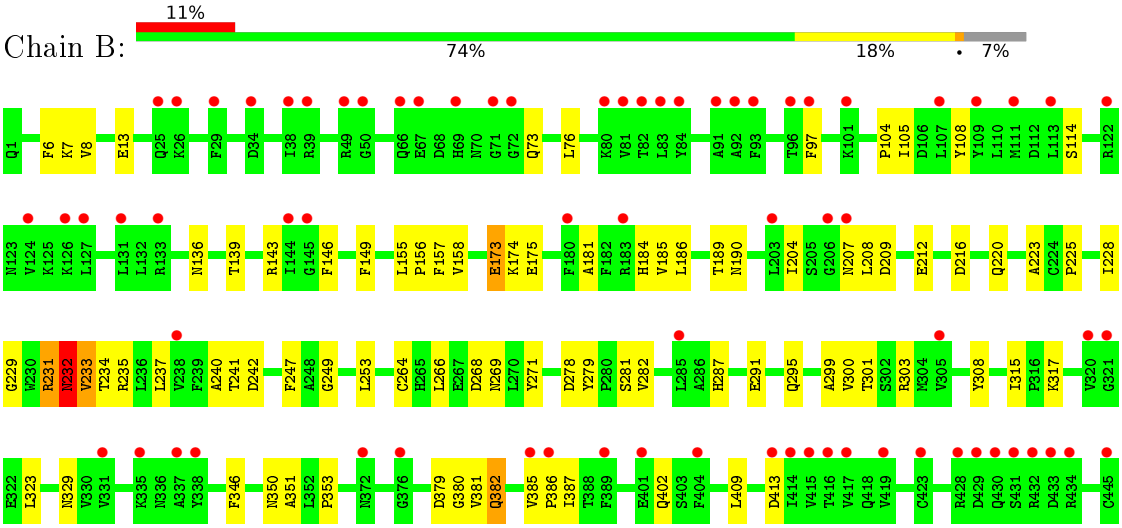
• Molecule 1: Integrin alpha-X

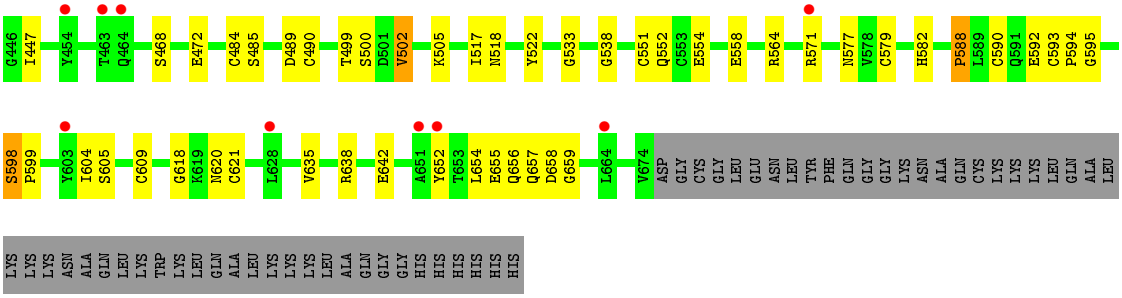
Chain G:





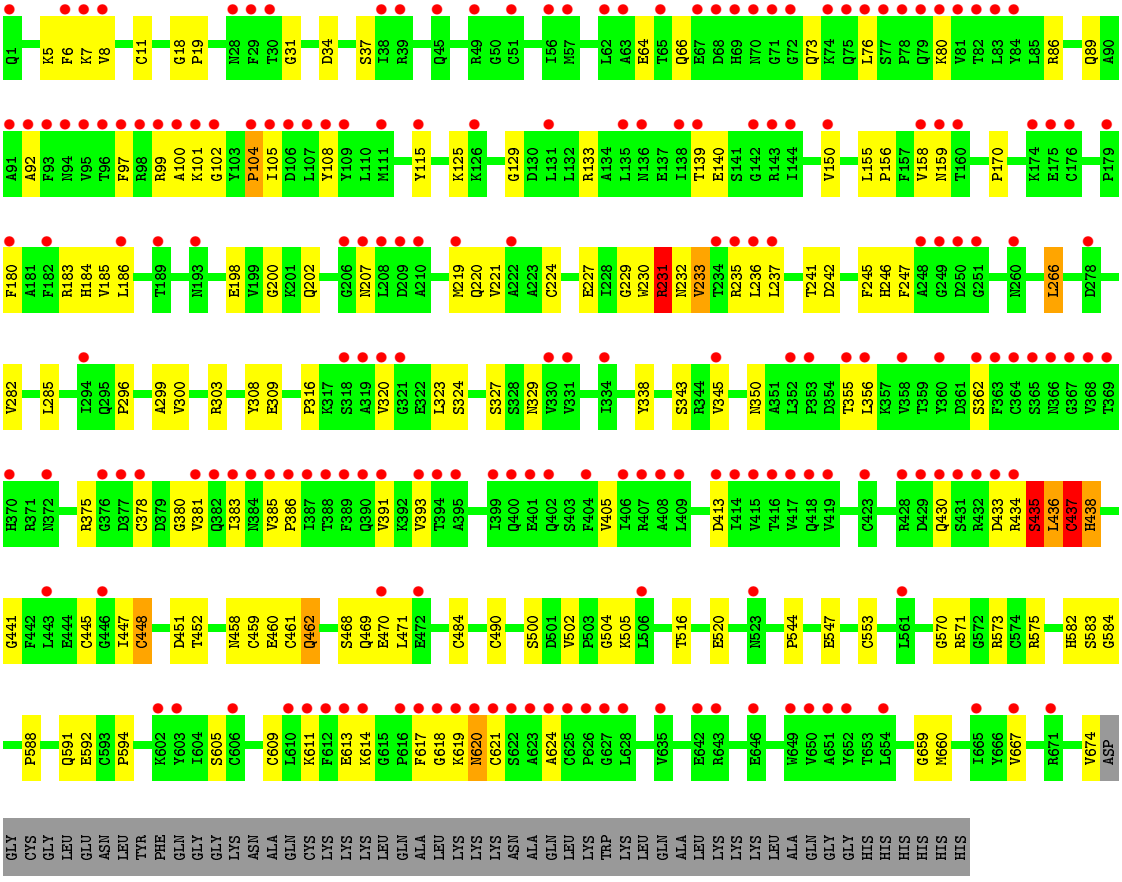
• Molecule 2: Integrin beta-2





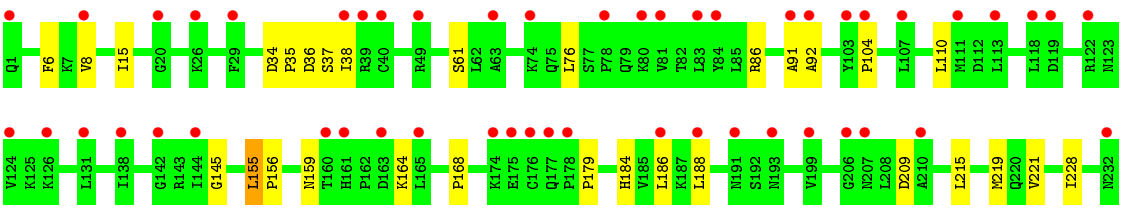
• Molecule 2: Integrin beta-2

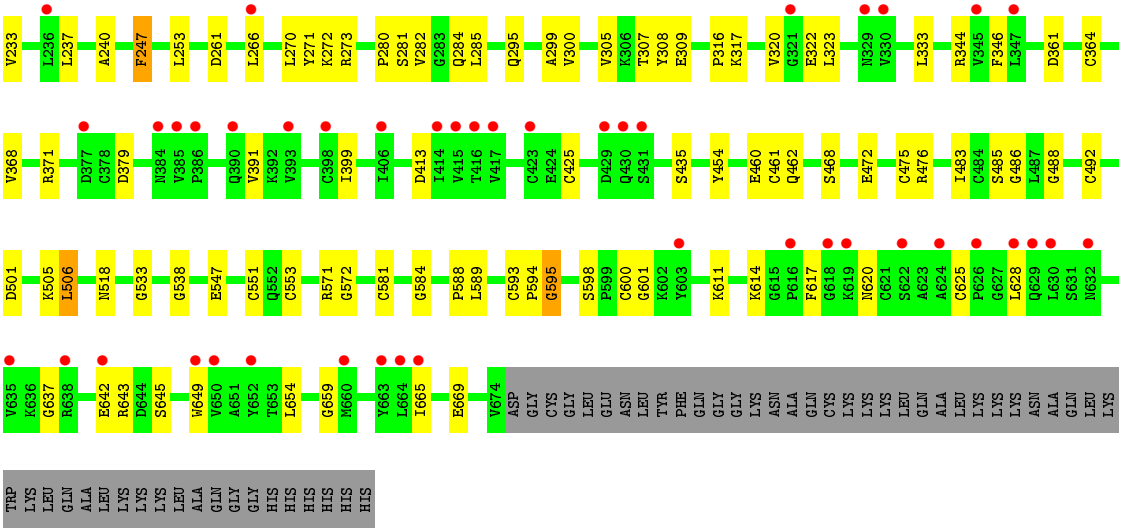
Chain D:



• Molecule 2: Integrin beta-2

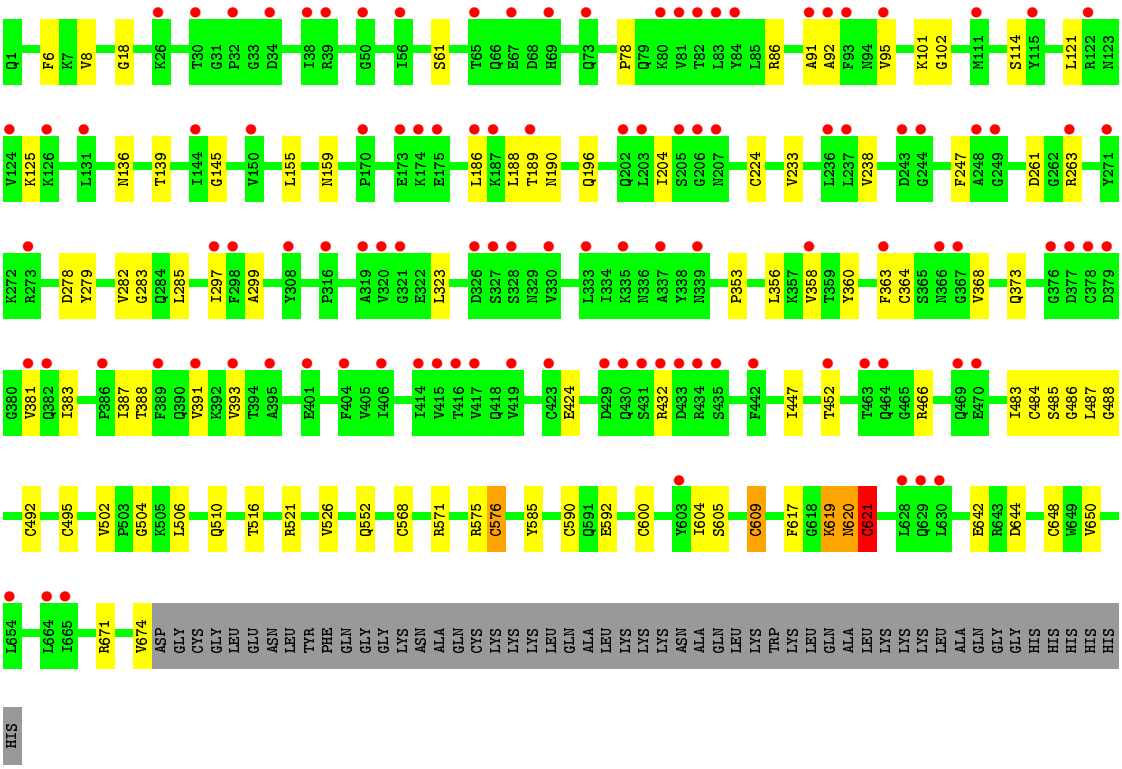
Chain F:





- Molecule 2: Integrin beta-2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.03Å 163.48Å 536.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 3.30 49.51 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.51-3.30) 97.0 (49.51-3.15)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.257 , 0.307 0.256 , 0.307	Depositor DCC
R_{free} test set	1813 reflections (1.04%)	DCC
Wilson B-factor (Å^2)	125.2	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 152.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	51071	wwPDB-VP
Average B, all atoms (Å^2)	200.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: MG, BMA, CA, NAG, 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	0.31	0/8557	0.58	2/11623 (0.0%)
1	C	0.35	1/6997 (0.0%)	0.60	2/9516 (0.0%)
1	E	0.31	0/7004	0.60	3/9526 (0.0%)
1	G	0.32	0/6941	0.60	3/9447 (0.0%)
2	B	0.31	0/5291	0.58	1/7144 (0.0%)
2	D	0.32	0/5274	0.59	2/7122 (0.0%)
2	F	0.29	0/5288	0.55	1/7140 (0.0%)
2	H	0.31	0/5280	0.56	2/7129 (0.0%)
All	All	0.32	1/50632 (0.0%)	0.58	16/68647 (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	4
1	C	0	6
1	E	0	3
1	G	0	3
2	B	0	2
2	D	0	5
All	All	0	23

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	722	LYS	C-N	11.19	1.55	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	448	CYS	CA-CB-SG	9.35	130.84	114.00
1	E	115	LEU	CA-CB-CG	8.01	133.71	115.30
2	H	432	ARG	NE-CZ-NH1	-7.32	116.64	120.30
2	D	266	LEU	CA-CB-CG	-6.69	99.91	115.30
1	A	663	ASP	CB-CG-OD1	6.29	123.96	118.30

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	480	ARG	Peptide
1	A	724	LEU	Peptide
1	A	82	SER	Peptide
1	A	885	ASN	Peptide
2	B	173	GLU	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	8371	0	8200	203	1
1	C	6834	0	6700	171	0
1	E	6838	0	6699	194	0
1	G	6787	0	6617	155	0
2	B	5191	0	4979	86	0
2	D	5178	0	4963	118	1
2	F	5189	0	4987	76	0
2	H	5184	0	4971	55	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
3	E	3	0	0	0	0
3	F	1	0	0	0	0
3	G	3	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
5	A	168	0	148	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	56	0	51	0	0
5	C	168	0	148	21	0
5	D	28	0	26	2	0
5	E	168	0	148	10	0
5	F	42	0	39	1	0
5	G	168	0	148	16	0
5	H	56	0	52	2	0
6	A	44	0	36	0	0
6	C	44	0	34	2	0
6	E	44	0	34	3	0
6	G	44	0	33	7	0
7	A	110	0	94	1	0
7	C	99	0	87	1	0
7	E	77	0	69	1	1
7	G	99	0	87	9	0
8	A	29	0	0	3	0
8	B	4	0	0	1	0
8	C	7	0	0	4	0
8	D	3	0	0	0	0
8	E	10	0	0	3	0
8	F	2	0	0	2	0
8	G	10	0	0	0	0
8	H	2	0	0	1	0
All	All	51071	0	49350	1016	2

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 10.

The worst 5 of 1016 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:308:ASN:HA	1:A:311:LYS:HD2	1.62	0.80
1:E:481:GLY:HA2	1:E:1021:GLN:HB2	1.66	0.76
1:A:438:TYR:HD1	1:A:441:ALA:HB2	1.54	0.73
1:E:919:LEU:HD21	1:E:930:HIS:HB3	1.70	0.73
2:D:99:ARG:NH2	2:D:338:TYR:OH	2.22	0.73

All (2) 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)
2:D:64:GLU:OE2	7:E:3719:MAN:O4[1_655]	2.02	0.18
1:A:192:ASN:ND2	1:A:986:PRO:O[4_455]	2.16	0.04

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	1078/1137 (95%)	958 (89%)	98 (9%)	22 (2%)	9	43
1	C	883/1137 (78%)	792 (90%)	68 (8%)	23 (3%)	7	36
1	E	884/1137 (78%)	791 (90%)	73 (8%)	20 (2%)	8	39
1	G	880/1137 (77%)	788 (90%)	71 (8%)	21 (2%)	7	38
2	B	673/727 (93%)	596 (89%)	71 (10%)	6 (1%)	21	60
2	D	672/727 (92%)	616 (92%)	47 (7%)	9 (1%)	15	52
2	F	673/727 (93%)	605 (90%)	60 (9%)	8 (1%)	16	54
2	H	672/727 (92%)	615 (92%)	47 (7%)	10 (2%)	13	49
All	All	6415/7456 (86%)	5761 (90%)	535 (8%)	119 (2%)	10	45

5 of 119 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	652	LEU
1	A	678	ASN
1	A	920	ASN
2	B	233	VAL
2	B	382	GLN

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	922/969 (95%)	910 (99%)	12 (1%)	76	89
1	C	756/969 (78%)	744 (98%)	12 (2%)	70	87
1	E	756/969 (78%)	739 (98%)	17 (2%)	60	84
1	G	748/969 (77%)	732 (98%)	16 (2%)	61	84
2	B	584/625 (93%)	577 (99%)	7 (1%)	78	90
2	D	582/625 (93%)	574 (99%)	8 (1%)	74	88
2	F	584/625 (93%)	580 (99%)	4 (1%)	88	94
2	H	583/625 (93%)	578 (99%)	5 (1%)	84	92
All	All	5515/6376 (86%)	5434 (98%)	81 (2%)	72	88

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	445	CYS
1	E	644	LYS
1	G	939	ASN
2	D	462	GLN
1	E	388	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	590	GLN
1	E	410	HIS
1	G	1066	GLN
1	C	930	HIS
2	D	89	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 129 ligands modelled in this entry, 17 are monoatomic - leaving 112 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	$\#\|Z\| > 2$
5	NAG	A	3031	1	14,14,15	0.26	0	15,19,21	0.45	0
5	NAG	A	3042	1	14,14,15	0.72	1 (7%)	15,19,21	1.45	1 (6%)
5	NAG	A	3070	1,5	14,14,15	0.30	0	15,19,21	0.63	0
5	NAG	A	3071	5,6	14,14,15	0.42	0	15,19,21	1.58	5 (33%)
6	BMA	A	3072	5,7	11,11,12	1.84	3 (27%)	15,15,17	2.93	4 (26%)
7	MAN	A	3073	7,6	11,11,12	0.74	0	15,15,17	1.56	4 (26%)
7	MAN	A	3074	7	11,11,12	0.61	0	15,15,17	1.04	1 (6%)
5	NAG	A	3373	1,5	14,14,15	0.45	0	15,19,21	0.67	0
5	NAG	A	3374	5,6	14,14,15	1.08	1 (7%)	15,19,21	0.93	1 (6%)
6	BMA	A	3375	5,7	11,11,12	2.03	2 (18%)	15,15,17	2.12	3 (20%)
7	MAN	A	3376	7,6	11,11,12	1.80	3 (27%)	15,15,17	1.63	3 (20%)
7	MAN	A	3377	7	11,11,12	1.04	1 (9%)	15,15,17	1.04	1 (6%)
7	MAN	A	3378	7	11,11,12	0.72	0	15,15,17	0.95	1 (6%)
7	MAN	A	3379	7	11,11,12	1.07	1 (9%)	15,15,17	1.95	4 (26%)
7	MAN	A	3380	7,6	11,11,12	1.51	2 (18%)	15,15,17	1.10	2 (13%)
7	MAN	A	3381	7	11,11,12	0.72	0	15,15,17	1.22	2 (13%)
7	MAN	A	3382	7	11,11,12	0.94	1 (9%)	15,15,17	1.82	4 (26%)
5	NAG	A	3678	1	14,14,15	0.70	1 (7%)	15,19,21	0.63	0
5	NAG	A	3716	1,5	14,14,15	0.50	0	15,19,21	0.63	0
5	NAG	A	3717	5,6	14,14,15	0.42	0	15,19,21	0.73	0
6	BMA	A	3718	5,7	11,11,12	1.52	2 (18%)	15,15,17	2.76	3 (20%)
7	MAN	A	3719	6	11,11,12	0.72	0	15,15,17	1.67	3 (20%)
5	NAG	A	3880	1,5	14,14,15	0.63	1 (7%)	15,19,21	0.94	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	3881	5,6	14,14,15	0.42	0	15,19,21	0.44	0
6	BMA	A	3882	5	11,11,12	0.72	0	15,15,17	0.94	1 (6%)
5	NAG	A	3920	1	14,14,15	0.75	1 (7%)	15,19,21	0.50	0
5	NAG	B	3094	2,5	14,14,15	1.20	1 (7%)	15,19,21	1.78	5 (33%)
5	NAG	B	3095	5	14,14,15	0.21	0	15,19,21	0.25	0
5	NAG	B	3232	2	14,14,15	1.02	1 (7%)	15,19,21	1.75	2 (13%)
5	NAG	B	3620	2	14,14,15	0.43	0	15,19,21	0.41	0
5	NAG	C	3031	1	14,14,15	0.25	0	15,19,21	0.47	0
5	NAG	C	3042	1	14,14,15	1.08	2 (14%)	15,19,21	0.34	0
5	NAG	C	3070	1,5	14,14,15	1.13	1 (7%)	15,19,21	1.01	0
5	NAG	C	3071	5,6	14,14,15	0.84	1 (7%)	15,19,21	1.51	4 (26%)
6	BMA	C	3072	5,7	11,11,12	2.68	3 (27%)	15,15,17	1.74	4 (26%)
7	MAN	C	3073	6	11,11,12	0.81	0	15,15,17	1.07	2 (13%)
5	NAG	C	3373	1,5	14,14,15	0.78	1 (7%)	15,19,21	0.68	0
5	NAG	C	3374	5,6	14,14,15	0.67	0	15,19,21	1.87	4 (26%)
6	BMA	C	3375	5,7	11,11,12	2.25	4 (36%)	15,15,17	1.94	3 (20%)
7	MAN	C	3376	7,6	11,11,12	0.83	1 (9%)	15,15,17	0.98	2 (13%)
7	MAN	C	3377	7	11,11,12	1.94	4 (36%)	15,15,17	1.39	2 (13%)
7	MAN	C	3378	6	11,11,12	1.09	2 (18%)	15,15,17	1.36	3 (20%)
7	MAN	C	3380	7	11,11,12	1.02	1 (9%)	15,15,17	1.44	2 (13%)
5	NAG	C	3678	1	14,14,15	0.82	1 (7%)	15,19,21	1.36	2 (13%)
5	NAG	C	3716	1,5	14,14,15	0.73	1 (7%)	15,19,21	0.81	0
5	NAG	C	3717	5,6	14,14,15	0.44	0	15,19,21	1.39	1 (6%)
6	BMA	C	3718	5,7	11,11,12	0.70	0	15,15,17	1.08	2 (13%)
7	MAN	C	3719	7,6	11,11,12	1.25	2 (18%)	15,15,17	1.58	2 (13%)
7	MAN	C	3720	7	11,11,12	1.37	1 (9%)	15,15,17	0.99	1 (6%)
5	NAG	C	3880	1,5	14,14,15	0.48	0	15,19,21	1.21	1 (6%)
5	NAG	C	3881	5,6	14,14,15	0.54	0	15,19,21	0.46	0
6	BMA	C	3882	5,7	11,11,12	1.18	1 (9%)	15,15,17	1.06	1 (6%)
7	MAN	C	3883	6	11,11,12	0.56	0	15,15,17	2.20	3 (20%)
7	MAN	C	3884	6	11,11,12	1.72	4 (36%)	15,15,17	1.96	4 (26%)
5	NAG	C	3920	1	14,14,15	0.76	1 (7%)	15,19,21	0.86	0
5	NAG	D	3232	2	14,14,15	0.85	1 (7%)	15,19,21	0.81	0
5	NAG	D	3620	2	14,14,15	0.39	0	15,19,21	0.39	0
5	NAG	E	3031	1	14,14,15	0.33	0	15,19,21	0.37	0
5	NAG	E	3042	1	14,14,15	0.42	0	15,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	E	3070	1,5	14,14,15	0.78	1 (7%)	15,19,21	0.85	1 (6%)
5	NAG	E	3071	5,6	14,14,15	1.12	2 (14%)	15,19,21	1.08	2 (13%)
6	BMA	E	3072	5,7	11,11,12	2.26	6 (54%)	15,15,17	2.11	6 (40%)
7	MAN	E	3073	6	11,11,12	0.71	0	15,15,17	1.00	2 (13%)
7	MAN	E	3074	7,6	11,11,12	2.75	5 (45%)	15,15,17	1.43	3 (20%)
7	MAN	E	3075	7	11,11,12	0.79	0	15,15,17	1.00	1 (6%)
5	NAG	E	3373	1,5	14,14,15	0.68	0	15,19,21	0.73	1 (6%)
5	NAG	E	3374	5,6	14,14,15	0.30	0	15,19,21	0.34	0
6	BMA	E	3375	5,7	11,11,12	0.97	1 (9%)	15,15,17	1.24	3 (20%)
7	MAN	E	3380	6	11,11,12	0.68	0	15,15,17	1.55	4 (26%)
5	NAG	E	3678	1	14,14,15	0.35	0	15,19,21	1.12	1 (6%)
5	NAG	E	3716	1,5	14,14,15	0.91	1 (7%)	15,19,21	0.76	0
5	NAG	E	3717	5,6	14,14,15	0.72	1 (7%)	15,19,21	0.68	0
6	BMA	E	3718	5,7	11,11,12	0.98	1 (9%)	15,15,17	1.69	4 (26%)
7	MAN	E	3719	6	11,11,12	0.94	1 (9%)	15,15,17	0.90	1 (6%)
5	NAG	E	3880	1,5	14,14,15	1.13	1 (7%)	15,19,21	2.17	2 (13%)
5	NAG	E	3881	5,6	14,14,15	0.69	1 (7%)	15,19,21	0.92	1 (6%)
6	BMA	E	3882	5,7	11,11,12	1.72	3 (27%)	15,15,17	1.77	4 (26%)
7	MAN	E	3883	6	11,11,12	0.75	0	15,15,17	1.08	2 (13%)
7	MAN	E	3884	6	11,11,12	2.22	2 (18%)	15,15,17	1.99	3 (20%)
5	NAG	E	3920	1	14,14,15	0.73	1 (7%)	15,19,21	3.90	2 (13%)
5	NAG	F	3094	2	14,14,15	0.43	0	15,19,21	0.56	0
5	NAG	F	3190	2	14,14,15	0.34	0	15,19,21	0.90	1 (6%)
5	NAG	F	3620	2	14,14,15	0.54	0	15,19,21	0.44	0
5	NAG	G	3031	1	14,14,15	0.35	0	15,19,21	0.51	0
5	NAG	G	3042	1	14,14,15	0.80	1 (7%)	15,19,21	0.31	0
5	NAG	G	3070	1,5	14,14,15	0.51	0	15,19,21	1.17	0
5	NAG	G	3071	5,6	14,14,15	0.52	0	15,19,21	0.90	0
6	BMA	G	3072	5,7	11,11,12	0.78	0	15,15,17	1.20	1 (6%)
7	MAN	G	3073	6	11,11,12	0.94	1 (9%)	15,15,17	2.22	4 (26%)
7	MAN	G	3074	6	11,11,12	0.95	0	15,15,17	1.82	2 (13%)
5	NAG	G	3373	1,5	14,14,15	1.63	1 (7%)	15,19,21	0.89	1 (6%)
5	NAG	G	3374	5,6	14,14,15	0.65	0	15,19,21	1.25	2 (13%)
6	BMA	G	3375	5,7	11,11,12	1.49	3 (27%)	15,15,17	1.97	7 (46%)
7	MAN	G	3376	7,6	11,11,12	1.68	3 (27%)	15,15,17	1.51	1 (6%)
7	MAN	G	3377	7	11,11,12	0.78	0	15,15,17	1.32	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	G	3379	7,6	11,11,12	0.95	1 (9%)	15,15,17	1.11	2 (13%)
7	MAN	G	3380	7	11,11,12	0.69	0	15,15,17	1.41	3 (20%)
5	NAG	G	3678	1	14,14,15	0.72	1 (7%)	15,19,21	0.63	0
5	NAG	G	3716	1,5	14,14,15	0.51	0	15,19,21	0.94	1 (6%)
5	NAG	G	3717	5,6	14,14,15	0.78	1 (7%)	15,19,21	1.21	1 (6%)
6	BMA	G	3718	5,7	11,11,12	1.17	1 (9%)	15,15,17	1.36	2 (13%)
7	MAN	G	3719	6	11,11,12	1.04	1 (9%)	15,15,17	0.93	1 (6%)
5	NAG	G	3880	1,5	14,14,15	1.14	1 (7%)	15,19,21	1.15	2 (13%)
5	NAG	G	3881	5,6	14,14,15	0.73	1 (7%)	15,19,21	2.08	1 (6%)
6	BMA	G	3882	5,7	11,11,12	1.19	1 (9%)	15,15,17	0.97	1 (6%)
7	MAN	G	3883	7,6	11,11,12	0.79	1 (9%)	15,15,17	1.78	2 (13%)
7	MAN	G	3884	7	11,11,12	1.33	2 (18%)	15,15,17	1.64	4 (26%)
5	NAG	G	3920	1	14,14,15	0.89	1 (7%)	15,19,21	0.46	0
5	NAG	H	3094	2	14,14,15	0.56	1 (7%)	15,19,21	0.33	0
5	NAG	H	3190	2	14,14,15	1.15	1 (7%)	15,19,21	0.85	1 (6%)
5	NAG	H	3232	2	14,14,15	0.85	1 (7%)	15,19,21	2.48	2 (13%)
5	NAG	H	3620	2	14,14,15	0.38	0	15,19,21	0.78	1 (6%)

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
5	NAG	A	3031	1	-	0/6/23/26	0/1/1/1
5	NAG	A	3042	1	-	0/6/23/26	0/1/1/1
5	NAG	A	3070	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	3071	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	3072	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	3073	7,6	-	0/2/19/22	0/1/1/1
7	MAN	A	3074	7	-	0/2/19/22	0/1/1/1
5	NAG	A	3373	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	3374	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	3375	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	3376	7,6	-	0/2/19/22	0/1/1/1
7	MAN	A	3377	7	-	0/2/19/22	0/1/1/1
7	MAN	A	3378	7	-	0/2/19/22	0/1/1/1
7	MAN	A	3379	7	-	0/2/19/22	0/1/1/1
7	MAN	A	3380	7,6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	A	3381	7	-	0/2/19/22	0/1/1/1
7	MAN	A	3382	7	-	0/2/19/22	0/1/1/1
5	NAG	A	3678	1	-	0/6/23/26	0/1/1/1
5	NAG	A	3716	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	3717	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	3718	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	3719	6	-	0/2/19/22	0/1/1/1
5	NAG	A	3880	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	3881	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	3882	5	-	0/2/19/22	0/1/1/1
5	NAG	A	3920	1	-	0/6/23/26	0/1/1/1
5	NAG	B	3094	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	3095	5	-	0/6/23/26	0/1/1/1
5	NAG	B	3232	2	-	0/6/23/26	0/1/1/1
5	NAG	B	3620	2	-	0/6/23/26	0/1/1/1
5	NAG	C	3031	1	-	0/6/23/26	0/1/1/1
5	NAG	C	3042	1	-	0/6/23/26	0/1/1/1
5	NAG	C	3070	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	3071	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	3072	5,7	-	0/2/19/22	0/1/1/1
7	MAN	C	3073	6	-	0/2/19/22	0/1/1/1
5	NAG	C	3373	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	3374	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	3375	5,7	-	0/2/19/22	0/1/1/1
7	MAN	C	3376	7,6	-	0/2/19/22	0/1/1/1
7	MAN	C	3377	7	-	0/2/19/22	0/1/1/1
7	MAN	C	3378	6	-	0/2/19/22	0/1/1/1
7	MAN	C	3380	7	-	0/2/19/22	0/1/1/1
5	NAG	C	3678	1	-	0/6/23/26	0/1/1/1
5	NAG	C	3716	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	3717	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	3718	5,7	-	0/2/19/22	0/1/1/1
7	MAN	C	3719	7,6	-	0/2/19/22	0/1/1/1
7	MAN	C	3720	7	-	0/2/19/22	0/1/1/1
5	NAG	C	3880	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	3881	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	3882	5,7	-	0/2/19/22	0/1/1/1
7	MAN	C	3883	6	-	0/2/19/22	0/1/1/1
7	MAN	C	3884	6	-	0/2/19/22	0/1/1/1
5	NAG	C	3920	1	-	0/6/23/26	0/1/1/1
5	NAG	D	3232	2	-	0/6/23/26	0/1/1/1
5	NAG	D	3620	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	3031	1	-	0/6/23/26	0/1/1/1
5	NAG	E	3042	1	-	0/6/23/26	0/1/1/1
5	NAG	E	3070	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	3071	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	3072	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	3073	6	-	0/2/19/22	0/1/1/1
7	MAN	E	3074	7,6	-	0/2/19/22	0/1/1/1
7	MAN	E	3075	7	-	0/2/19/22	0/1/1/1
5	NAG	E	3373	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	3374	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	3375	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	3380	6	-	0/2/19/22	0/1/1/1
5	NAG	E	3678	1	-	0/6/23/26	0/1/1/1
5	NAG	E	3716	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	3717	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	3718	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	3719	6	-	0/2/19/22	0/1/1/1
5	NAG	E	3880	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	3881	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	3882	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	3883	6	-	0/2/19/22	0/1/1/1
7	MAN	E	3884	6	-	0/2/19/22	0/1/1/1
5	NAG	E	3920	1	-	0/6/23/26	0/1/1/1
5	NAG	F	3094	2	-	0/6/23/26	0/1/1/1
5	NAG	F	3190	2	-	0/6/23/26	0/1/1/1
5	NAG	F	3620	2	-	0/6/23/26	0/1/1/1
5	NAG	G	3031	1	-	0/6/23/26	0/1/1/1
5	NAG	G	3042	1	-	0/6/23/26	0/1/1/1
5	NAG	G	3070	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	3071	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	3072	5,7	-	0/2/19/22	0/1/1/1
7	MAN	G	3073	6	-	0/2/19/22	0/1/1/1
7	MAN	G	3074	6	-	0/2/19/22	0/1/1/1
5	NAG	G	3373	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	3374	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	3375	5,7	-	0/2/19/22	0/1/1/1
7	MAN	G	3376	7,6	-	0/2/19/22	0/1/1/1
7	MAN	G	3377	7	-	0/2/19/22	0/1/1/1
7	MAN	G	3379	7,6	-	0/2/19/22	0/1/1/1
7	MAN	G	3380	7	-	0/2/19/22	0/1/1/1
5	NAG	G	3678	1	-	0/6/23/26	0/1/1/1
5	NAG	G	3716	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	3717	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	3718	5,7	-	0/2/19/22	0/1/1/1
7	MAN	G	3719	6	-	0/2/19/22	0/1/1/1
5	NAG	G	3880	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	3881	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	3882	5,7	-	0/2/19/22	0/1/1/1
7	MAN	G	3883	7,6	-	0/2/19/22	0/1/1/1
7	MAN	G	3884	7	-	0/2/19/22	0/1/1/1
5	NAG	G	3920	1	-	0/6/23/26	0/1/1/1
5	NAG	H	3094	2	-	0/6/23/26	0/1/1/1
5	NAG	H	3190	2	-	0/6/23/26	0/1/1/1
5	NAG	H	3232	2	-	0/6/23/26	0/1/1/1
5	NAG	H	3620	2	-	0/6/23/26	0/1/1/1

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3072	BMA	O5-C1	-6.81	1.32	1.43
5	G	3373	NAG	O5-C1	-5.92	1.34	1.43
6	A	3375	BMA	O5-C1	-5.41	1.34	1.43
6	A	3072	BMA	O5-C1	-4.76	1.36	1.43
7	A	3376	MAN	O5-C1	-4.52	1.36	1.43

The worst 5 of 182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	3072	BMA	C1-C2-C3	-8.99	98.66	109.55
6	A	3718	BMA	C1-C2-C3	-7.55	100.41	109.55
6	A	3718	BMA	C1-O5-C5	-6.06	103.22	112.14
6	A	3072	BMA	C1-O5-C5	-5.22	104.46	112.14
5	B	3232	NAG	C1-O5-C5	-4.96	104.85	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

53 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3031	NAG	1	0
5	A	3070	NAG	4	0
5	A	3071	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3374	NAG	1	0
7	A	3381	MAN	1	0
5	A	3716	NAG	2	0
5	A	3717	NAG	2	0
5	A	3880	NAG	2	0
5	A	3920	NAG	2	0
5	C	3031	NAG	1	0
5	C	3042	NAG	1	0
5	C	3070	NAG	3	0
5	C	3071	NAG	2	0
5	C	3373	NAG	3	0
5	C	3374	NAG	2	0
6	C	3375	BMA	2	0
7	C	3378	MAN	1	0
5	C	3716	NAG	3	0
5	C	3717	NAG	1	0
5	C	3880	NAG	1	0
5	C	3920	NAG	5	0
5	D	3232	NAG	1	0
5	D	3620	NAG	1	0
5	E	3070	NAG	1	0
6	E	3072	BMA	1	0
7	E	3074	MAN	1	0
5	E	3373	NAG	4	0
5	E	3717	NAG	3	0
6	E	3718	BMA	2	0
7	E	3719	MAN	0	1
5	E	3880	NAG	1	0
5	E	3920	NAG	1	0
5	F	3094	NAG	1	0
5	G	3042	NAG	3	0
5	G	3070	NAG	5	0
5	G	3071	NAG	2	0
6	G	3072	BMA	2	0
7	G	3074	MAN	2	0
6	G	3375	BMA	3	0
7	G	3376	MAN	2	0
7	G	3379	MAN	1	0
7	G	3380	MAN	2	0
5	G	3716	NAG	3	0
6	G	3718	BMA	1	0
7	G	3719	MAN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	3880	NAG	2	0
5	G	3881	NAG	2	0
6	G	3882	BMA	1	0
7	G	3883	MAN	1	0
7	G	3884	MAN	1	0
5	G	3920	NAG	2	0
5	H	3094	NAG	1	0
5	H	3232	NAG	1	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

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^{th} 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	1080/1137 (94%)	0.21	42 (3%) 43 36	86, 154, 247, 360	0
1	C	884/1137 (77%)	0.63	98 (11%) 7 6	90, 184, 288, 417	0
1	E	884/1137 (77%)	0.32	54 (6%) 25 20	84, 163, 267, 405	0
1	G	883/1137 (77%)	0.28	39 (4%) 38 31	86, 148, 255, 387	0
2	B	674/727 (92%)	0.59	81 (12%) 6 5	120, 217, 318, 438	0
2	D	674/727 (92%)	1.42	199 (29%) 1 1	136, 266, 376, 453	0
2	F	674/727 (92%)	0.67	94 (13%) 4 3	105, 213, 308, 375	0
2	H	674/727 (92%)	0.78	109 (16%) 3 2	101, 222, 327, 434	0
All	All	6427/7456 (86%)	0.57	716 (11%) 7 6	84, 188, 313, 453	0

The worst 5 of 716 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	433	ASP	19.9
2	D	92	ALA	19.3
2	B	92	ALA	16.3
2	D	91	ALA	16.2
2	D	82	THR	14.6

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 (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, 95^{th} 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
5	NAG	H	3620	14/15	0.78	0.62	6.17	203,255,288,311	0
5	NAG	G	3070	14/15	0.91	0.28	1.36	208,268,306,312	0
5	NAG	A	3373	14/15	0.85	0.38	1.28	214,248,299,302	0
5	NAG	C	3373	14/15	0.37	0.36	0.90	257,282,326,328	0
5	NAG	G	3031	14/15	0.84	0.23	0.83	139,227,255,259	0
5	NAG	F	3620	14/15	0.67	0.56	0.69	281,300,312,313	0
5	NAG	C	3920	14/15	0.61	0.48	0.62	261,304,317,320	0
5	NAG	G	3880	14/15	0.84	0.27	0.56	162,214,255,297	0
5	NAG	E	3716	14/15	0.96	0.21	0.48	92,173,221,231	0
5	NAG	G	3373	14/15	0.86	0.29	0.43	253,265,294,302	0
3	CA	A	2005	1/1	0.65	0.15	0.03	282,282,282,282	0
5	NAG	E	3373	14/15	0.85	0.25	-0.02	222,248,291,302	0
7	MAN	A	3382	11/12	0.81	0.18	-0.03	219,247,260,292	0
5	NAG	C	3880	14/15	0.80	0.20	-0.13	167,216,284,298	0
5	NAG	E	3070	14/15	0.73	0.30	-0.23	212,243,256,277	0
5	NAG	E	3880	14/15	0.93	0.22	-0.24	194,219,246,273	0
5	NAG	C	3070	14/15	0.54	0.25	-0.26	220,240,264,265	0
5	NAG	C	3031	14/15	0.88	0.21	-0.32	200,248,281,285	0
5	NAG	G	3920	14/15	0.80	0.29	-0.44	152,193,229,237	0
3	CA	D	2002	1/1	0.73	0.16	-0.45	715,715,715,715	0
5	NAG	D	3232	14/15	0.51	0.42	-0.47	220,239,242,244	0
5	NAG	C	3716	14/15	0.95	0.16	-0.53	116,173,218,249	0
3	CA	E	2007	1/1	0.88	0.18	-0.53	246,246,246,246	0
3	CA	C	2006	1/1	0.92	0.15	-0.54	232,232,232,232	0
5	NAG	A	3070	14/15	0.91	0.18	-0.61	182,238,254,256	0
5	NAG	G	3716	14/15	0.88	0.17	-0.72	130,217,244,263	0
5	NAG	A	3920	14/15	0.75	0.23	-0.80	165,310,345,346	0
3	CA	B	2002	1/1	0.93	0.14	-0.85	457,457,457,457	0
3	CA	G	2006	1/1	0.74	0.18	-0.93	214,214,214,214	0
5	NAG	A	3031	14/15	0.87	0.15	-0.98	126,244,266,274	0
5	NAG	E	3920	14/15	0.76	0.22	-0.99	230,286,310,319	0
3	CA	H	2002	1/1	0.87	0.09	-1.09	448,448,448,448	0
4	MG	A	2009	1/1	0.97	0.07	-1.09	370,370,370,370	0
5	NAG	H	3094	14/15	0.78	0.21	-1.11	239,260,312,313	0
3	CA	E	2006	1/1	0.81	0.13	-1.12	242,242,242,242	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CA	G	2007	1/1	0.96	0.10	-1.19	189,189,189,189	0
3	CA	G	2005	1/1	0.97	0.09	-1.37	240,240,240,240	0
5	NAG	A	3716	14/15	0.94	0.10	-1.40	105,177,205,238	0
5	NAG	E	3031	14/15	0.86	0.16	-1.45	172,223,244,254	0
3	CA	A	2006	1/1	0.86	0.07	-2.08	234,234,234,234	0
3	CA	E	2005	1/1	0.88	0.07	-2.14	276,276,276,276	0
3	CA	C	2007	1/1	0.71	0.05	-2.29	311,311,311,311	0
3	CA	A	2007	1/1	0.79	0.04	-2.32	238,238,238,238	0
3	CA	C	2005	1/1	0.97	0.04	-2.40	236,236,236,236	0
7	MAN	C	3884	11/12	0.85	0.29	-	205,224,243,264	0
5	NAG	C	3374	14/15	0.42	0.35	-	229,298,329,346	0
7	MAN	A	3377	11/12	0.74	0.36	-	308,325,333,336	0
6	BMA	C	3375	11/12	0.65	0.31	-	336,352,372,394	0
6	BMA	A	3375	11/12	0.76	0.15	-	260,272,289,292	0
5	NAG	G	3717	14/15	0.83	0.20	-	260,287,322,339	0
7	MAN	A	3380	11/12	0.89	0.19	-	253,283,295,302	0
7	MAN	E	3719	11/12	0.69	0.17	-	268,299,311,315	0
7	MAN	E	3075	11/12	0.80	0.91	-	214,236,249,250	0
6	BMA	E	3718	11/12	0.63	0.14	-	329,335,342,344	0
7	MAN	E	3074	11/12	0.74	0.70	-	243,252,266,272	0
5	NAG	A	3880	14/15	0.86	0.24	-	213,237,268,301	0
5	NAG	A	3071	14/15	0.86	0.15	-	201,244,258,278	0
7	MAN	E	3883	11/12	0.60	0.47	-	246,284,314,321	0
5	NAG	A	3881	14/15	0.65	0.28	-	225,301,319,329	0
5	NAG	A	3374	14/15	0.86	0.29	-	230,288,304,324	0
6	BMA	E	3882	11/12	0.73	0.28	-	260,320,325,331	0
5	NAG	B	3094	14/15	0.74	0.29	-	252,275,300,325	0
5	NAG	C	3042	14/15	0.75	0.63	-	195,241,267,281	0
3	CA	F	2002	1/1	0.94	0.13	-	505,505,505,505	0
7	MAN	G	3073	11/12	0.75	0.25	-	263,276,302,308	0
5	NAG	G	3071	14/15	0.86	0.18	-	225,265,287,289	0
7	MAN	C	3380	11/12	0.50	0.55	-	274,292,298,299	0
7	MAN	E	3380	11/12	0.77	0.28	-	269,325,347,348	0
5	NAG	C	3881	14/15	0.72	0.24	-	261,295,308,310	0
7	MAN	A	3381	11/12	0.86	0.29	-	269,291,305,306	0
7	MAN	G	3379	11/12	0.75	0.38	-	309,319,344,347	0
5	NAG	G	3881	14/15	0.38	0.45	-	239,315,332,345	0
6	BMA	C	3718	11/12	0.70	0.31	-	305,318,338,338	0
6	BMA	A	3718	11/12	0.64	0.44	-	313,322,328,341	0
5	NAG	G	3042	14/15	0.82	0.29	-	206,259,269,270	0
6	BMA	A	3072	11/12	0.76	0.23	-	291,299,315,325	0
7	MAN	C	3719	11/12	0.77	0.26	-	287,306,320,322	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	MAN	C	3377	11/12	0.69	0.48	-	273,287,297,298	0
7	MAN	A	3074	11/12	0.67	0.26	-	261,289,311,344	0
5	NAG	B	3095	14/15	0.87	0.64	-	273,334,340,343	0
7	MAN	G	3883	11/12	0.82	0.21	-	217,278,294,299	0
7	MAN	G	3074	11/12	0.73	0.21	-	237,293,323,332	0
6	BMA	G	3718	11/12	0.47	0.28	-	337,345,352,353	0
5	NAG	E	3881	14/15	0.74	0.40	-	285,304,339,371	0
5	NAG	B	3232	14/15	0.71	0.32	-	192,229,251,259	0
7	MAN	G	3376	11/12	0.59	0.51	-	346,370,378,391	0
6	BMA	G	3375	11/12	0.69	0.29	-	328,334,347,350	0
7	MAN	C	3376	11/12	0.02	0.26	-	288,304,311,317	0
6	BMA	C	3072	11/12	0.26	0.36	-	297,334,341,350	0
5	NAG	E	3042	14/15	0.71	0.34	-	205,258,290,292	0
5	NAG	A	3717	14/15	0.87	0.28	-	271,296,314,323	0
6	BMA	E	3072	11/12	0.83	0.47	-	274,304,315,326	0
5	NAG	C	3717	14/15	0.86	0.24	-	276,297,343,352	0
7	MAN	A	3378	11/12	0.63	0.43	-	263,300,333,333	0
7	MAN	G	3377	11/12	0.73	0.62	-	307,322,345,358	0
5	NAG	G	3374	14/15	0.84	0.30	-	242,271,298,315	0
5	NAG	A	3042	14/15	0.77	0.30	-	237,241,277,278	0
6	BMA	G	3072	11/12	0.80	0.21	-	310,323,330,334	0
7	MAN	C	3883	11/12	0.79	0.75	-	249,281,295,299	0
5	NAG	C	3071	14/15	0.72	0.28	-	219,269,303,323	0
5	NAG	B	3620	14/15	0.85	0.47	-	221,253,270,280	0
5	NAG	G	3678	14/15	0.76	0.33	-	196,238,257,263	0
5	NAG	H	3232	14/15	0.69	0.35	-	189,210,226,226	0
7	MAN	G	3380	11/12	0.63	0.20	-	230,289,305,305	0
7	MAN	E	3884	11/12	0.88	0.26	-	200,226,241,242	0
7	MAN	C	3378	11/12	0.81	0.37	-	317,336,352,359	0
6	BMA	A	3882	11/12	0.46	0.48	-	252,306,330,335	0
7	MAN	A	3073	11/12	0.87	0.25	-	282,287,289,290	0
7	MAN	C	3720	11/12	0.80	0.34	-	186,218,245,252	0
7	MAN	C	3073	11/12	0.72	0.36	-	251,320,334,336	0
5	NAG	F	3190	14/15	0.63	0.33	-	235,263,275,278	0
5	NAG	E	3678	14/15	0.79	0.28	-	188,244,283,300	0
5	NAG	F	3094	14/15	0.85	0.35	-	221,279,292,292	0
5	NAG	E	3374	14/15	0.82	0.34	-	233,292,313,337	0
5	NAG	A	3678	14/15	0.89	0.16	-	162,236,250,253	0
5	NAG	E	3071	14/15	0.91	0.23	-	219,262,289,297	0
7	MAN	A	3719	11/12	0.83	0.49	-	265,290,297,302	0
5	NAG	D	3620	14/15	0.50	0.85	-	259,279,292,296	0
7	MAN	G	3884	11/12	0.83	0.13	-	178,213,255,260	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	BMA	C	3882	11/12	0.73	0.29	-	287,305,328,361	0
7	MAN	A	3379	11/12	0.82	0.41	-	280,311,318,330	0
5	NAG	C	3678	14/15	0.83	0.34	-	225,273,310,321	0
5	NAG	E	3717	14/15	0.91	0.17	-	233,281,330,342	0
7	MAN	G	3719	11/12	0.70	0.36	-	270,309,322,327	0
6	BMA	E	3375	11/12	0.68	0.34	-	320,330,340,343	0
7	MAN	A	3376	11/12	0.73	0.24	-	309,311,326,327	0
6	BMA	G	3882	11/12	0.39	0.34	-	261,315,353,371	0
5	NAG	H	3190	14/15	0.81	0.17	-	215,264,276,276	0
7	MAN	E	3073	11/12	0.74	0.33	-	230,277,297,301	0

6.5 Other polymers (i)

There are no such residues in this entry.