Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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:

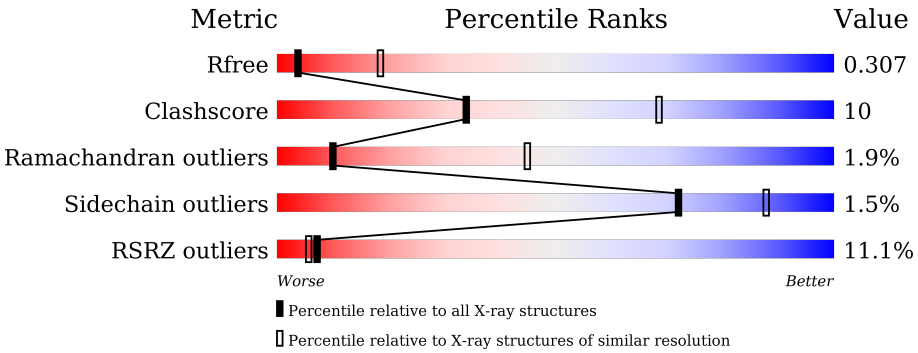
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	13% 76% 16% • 7%
2	H	727	15% 80% 12% • 7%

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

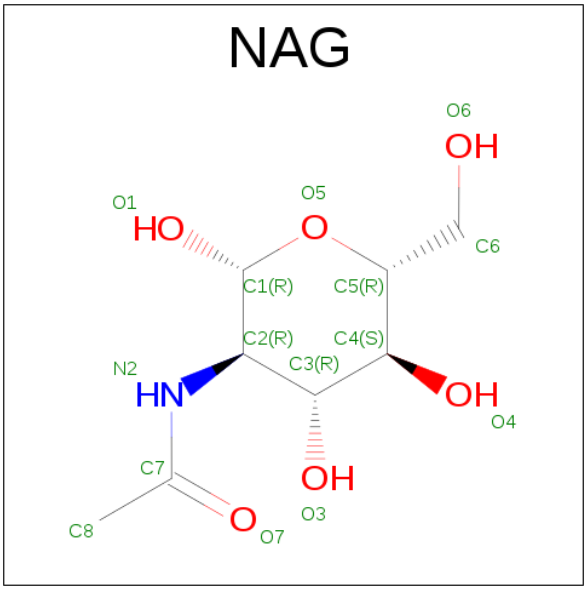
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0

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

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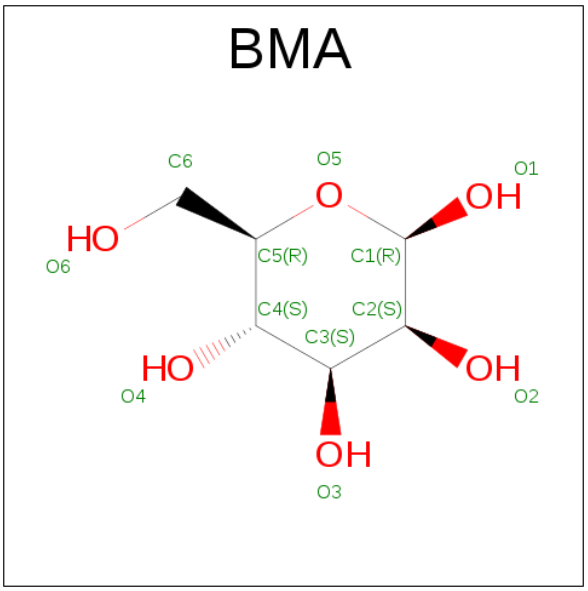
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total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

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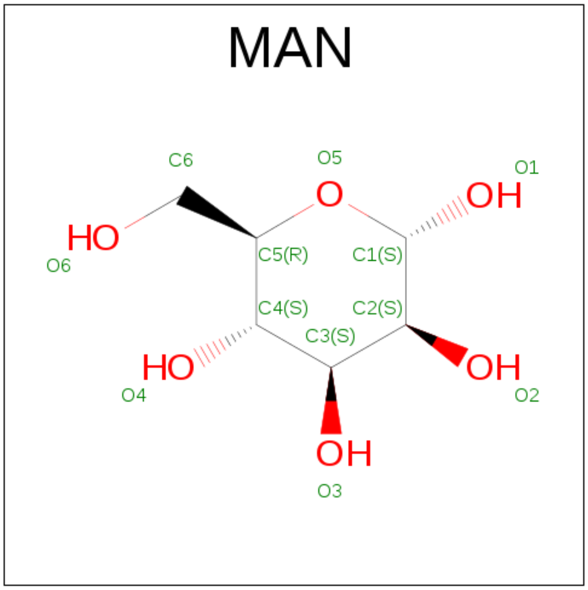
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C O 11 6 5	0	0
6	G	1	Total C O 11 6 5	0	0

- 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	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

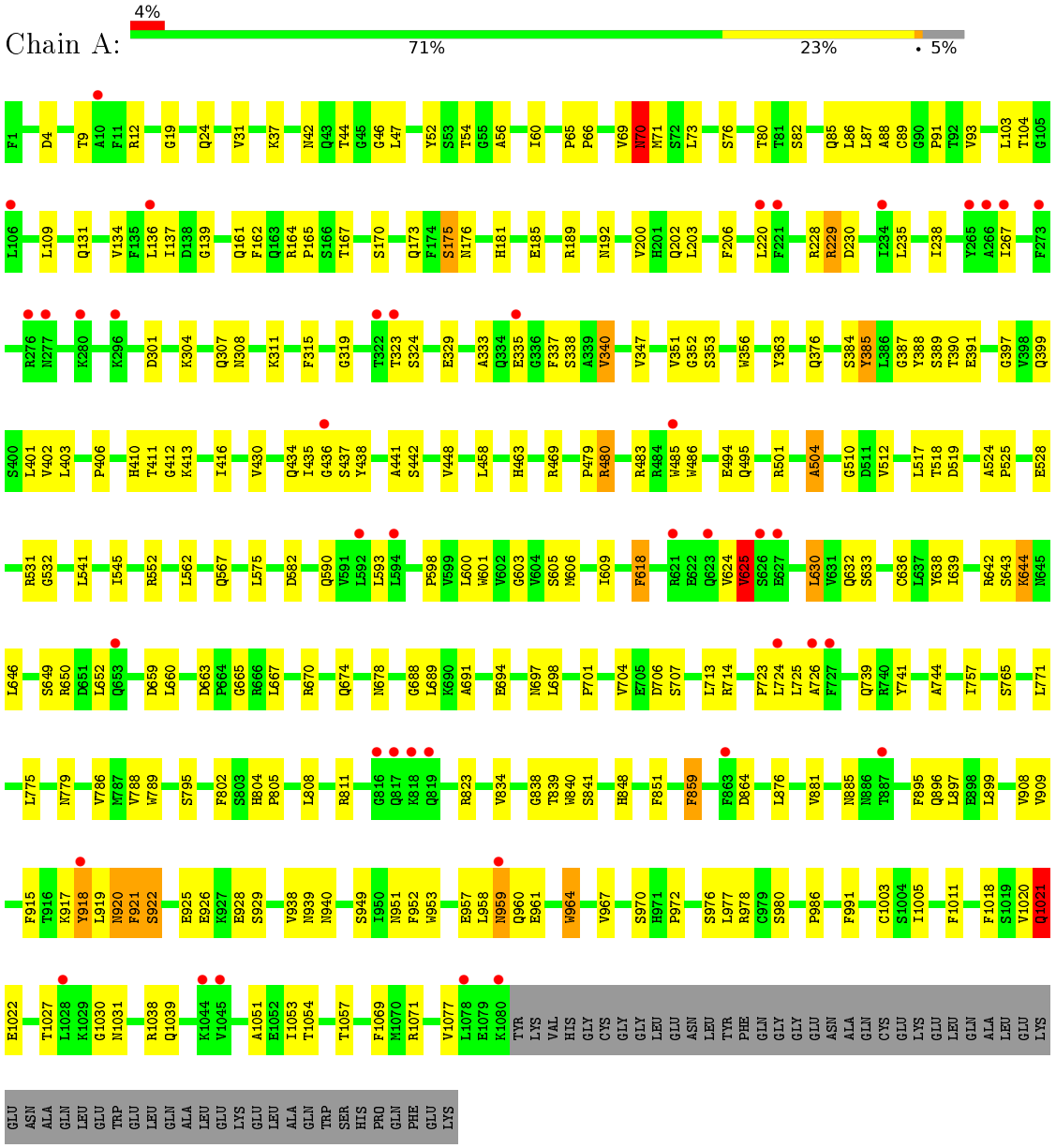
- Molecule 8 is water.

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)

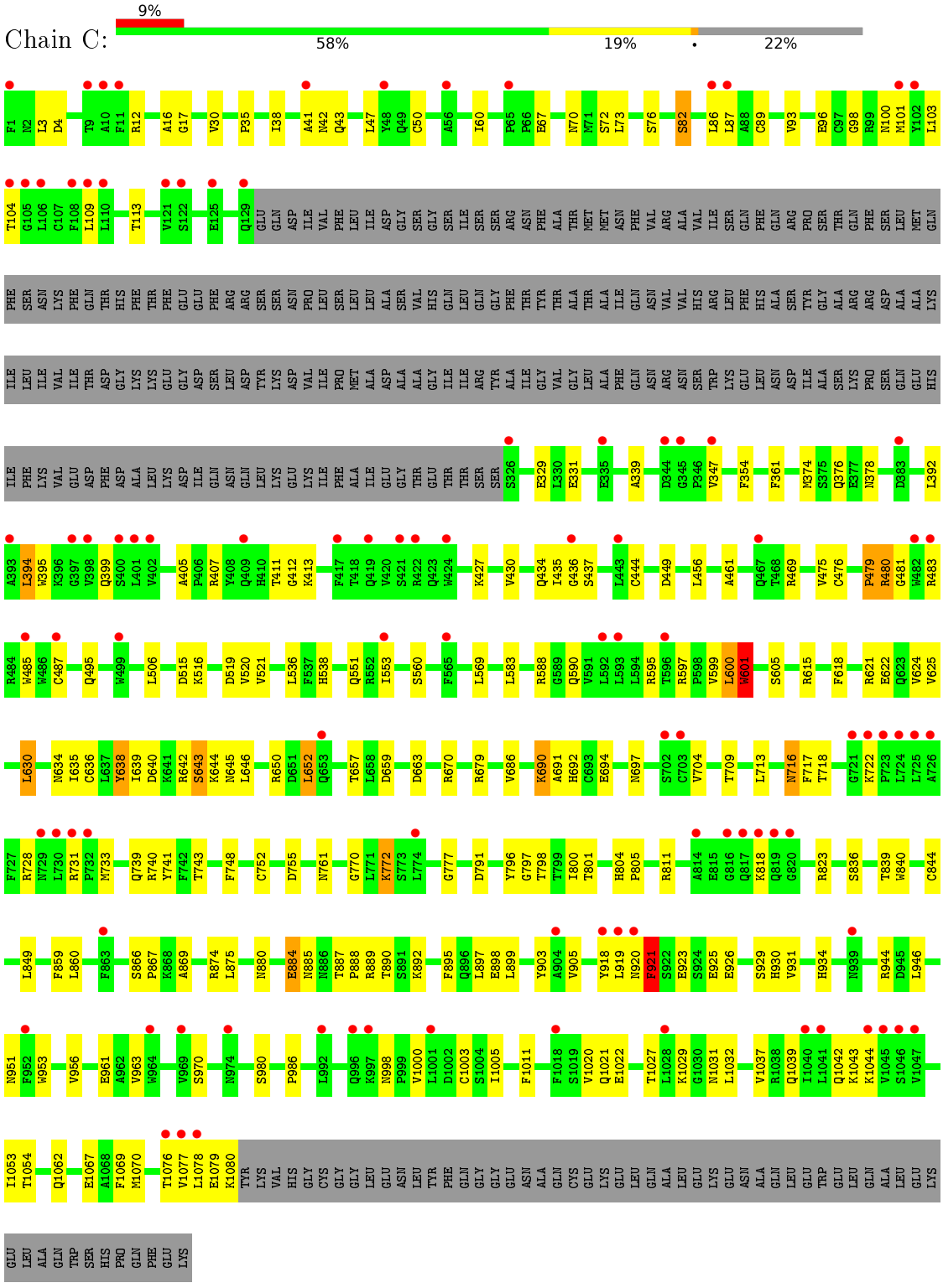
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



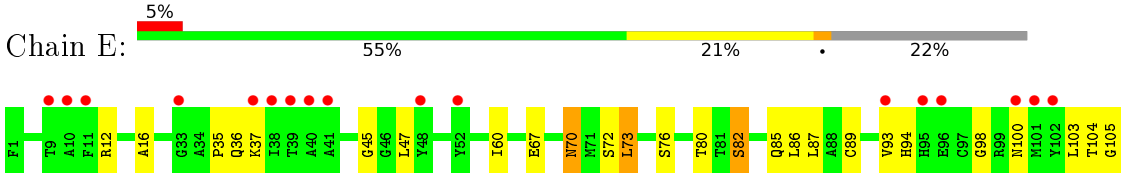
- Molecule 1: Integrin alpha-X

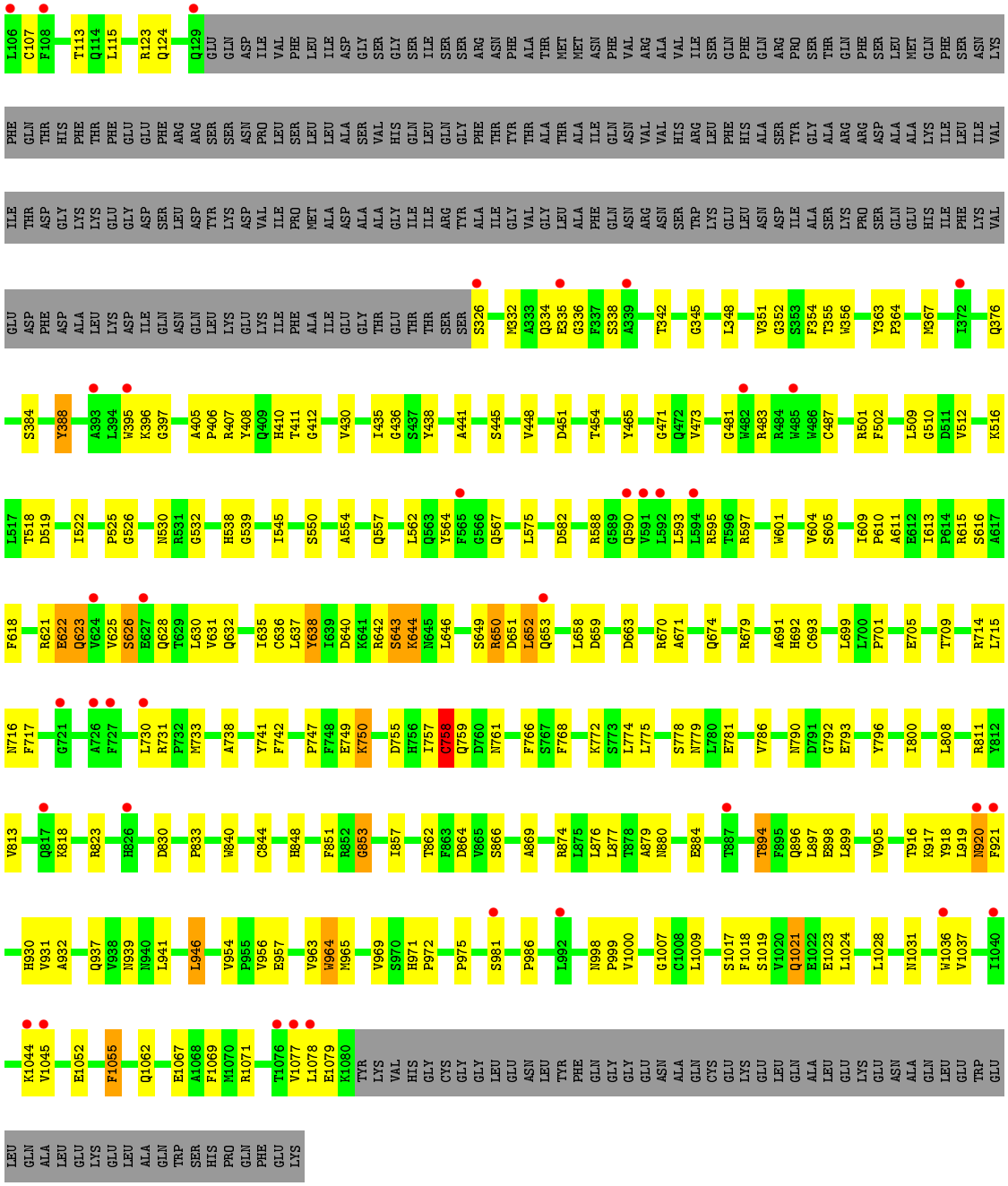
Chain C:



• Molecule 1: Integrin alpha-X

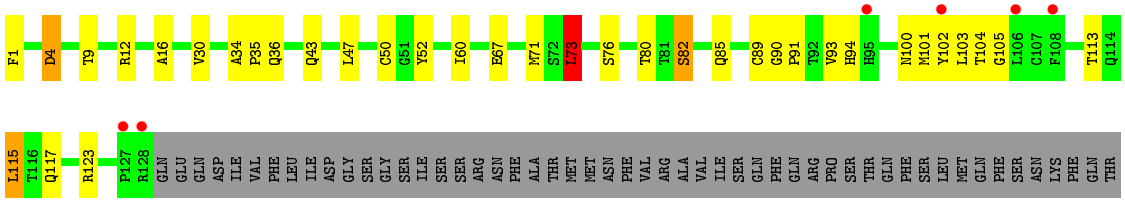
Chain E:

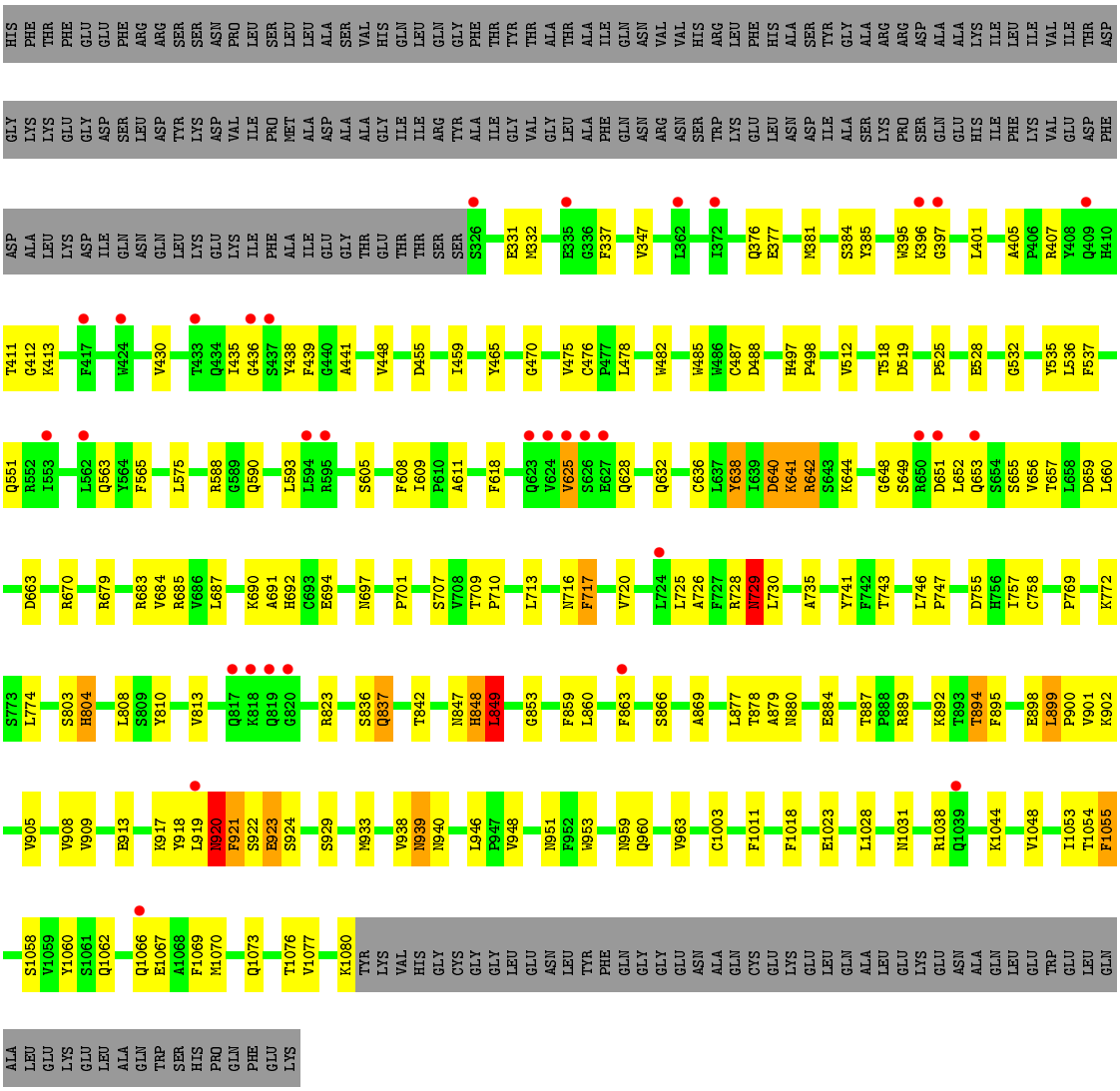




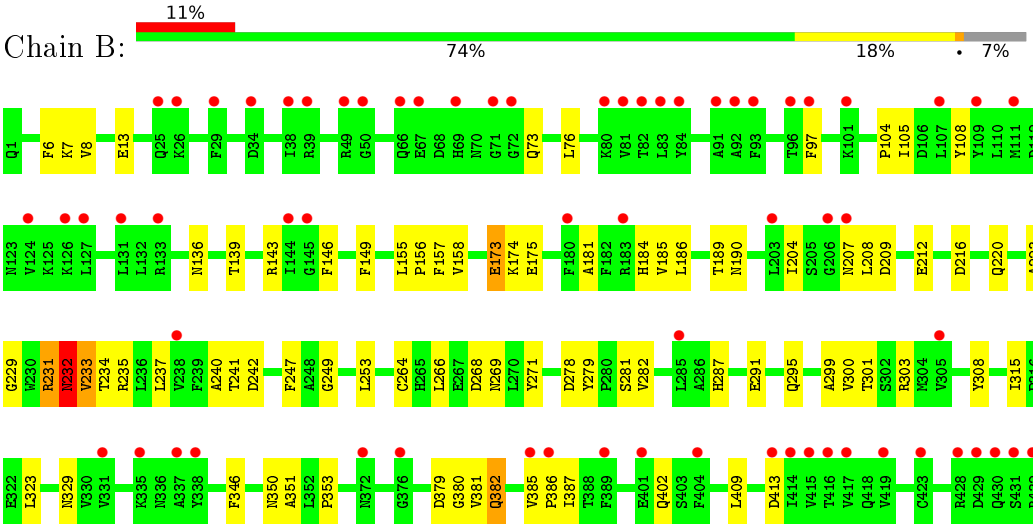
• Molecule 1: Integrin alpha-X

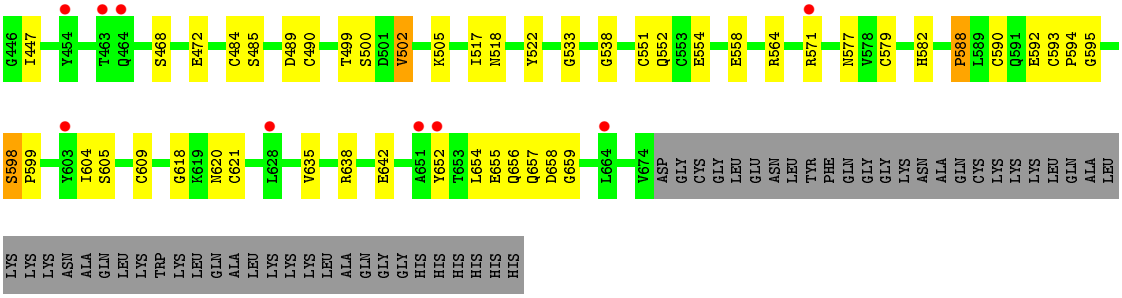
Chain G:





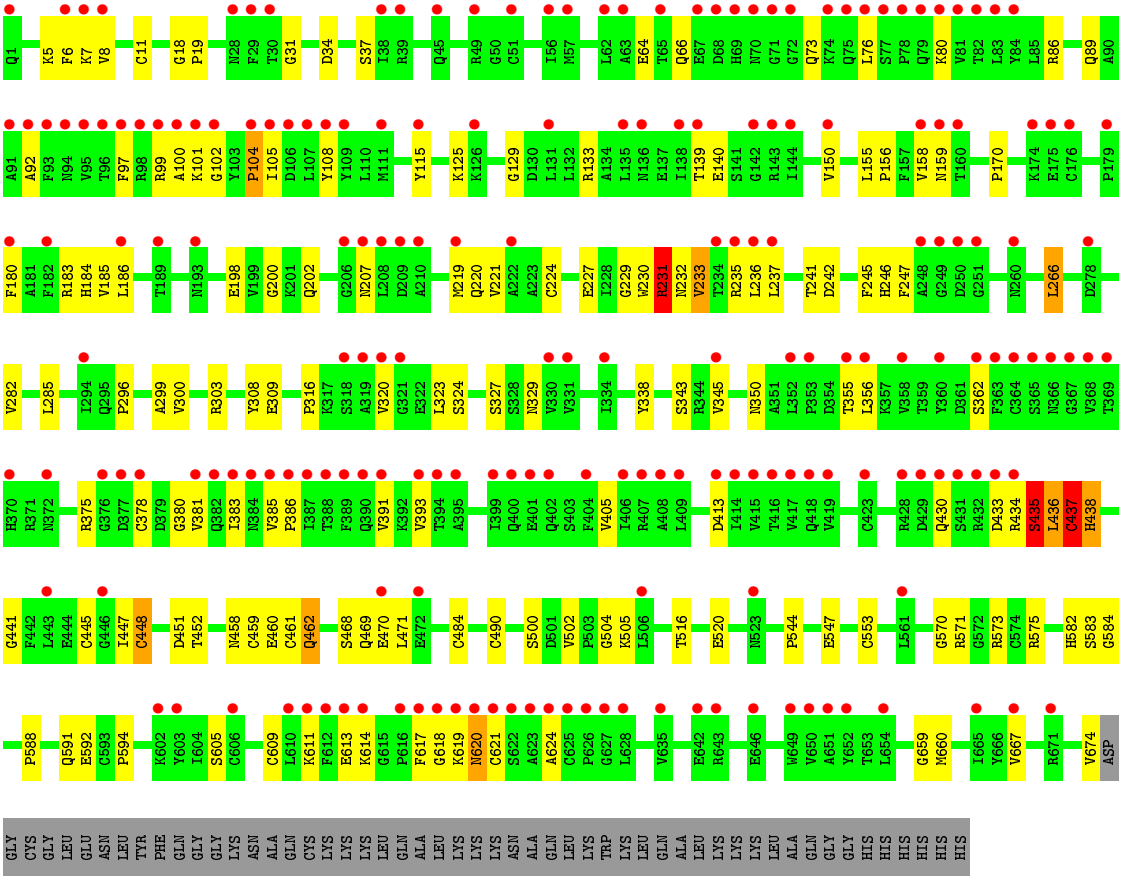
• Molecule 2: Integrin beta-2





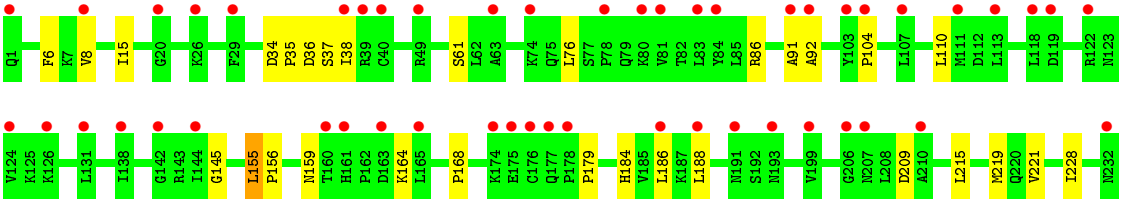
• Molecule 2: Integrin beta-2

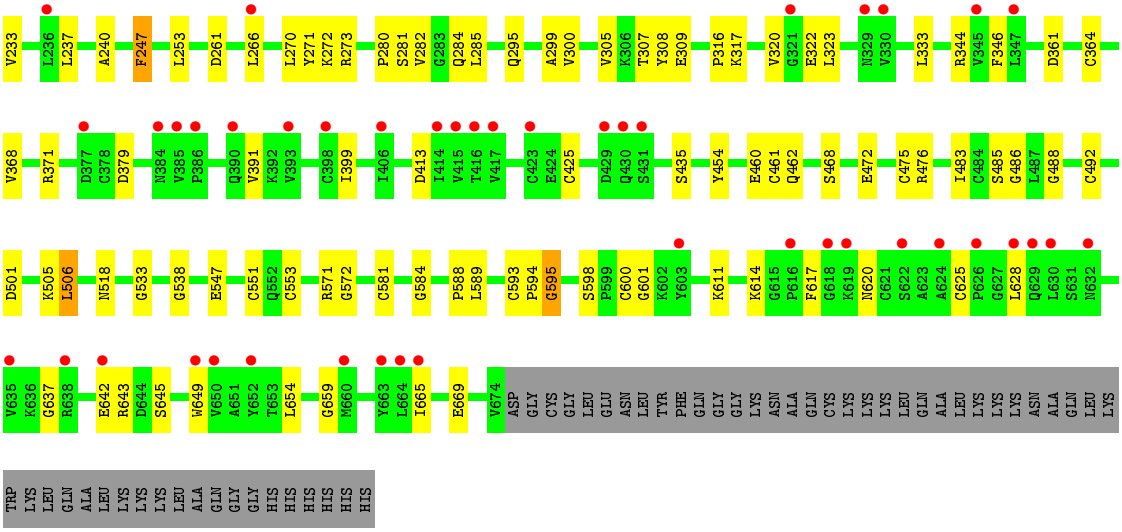
Chain D:



• Molecule 2: Integrin beta-2

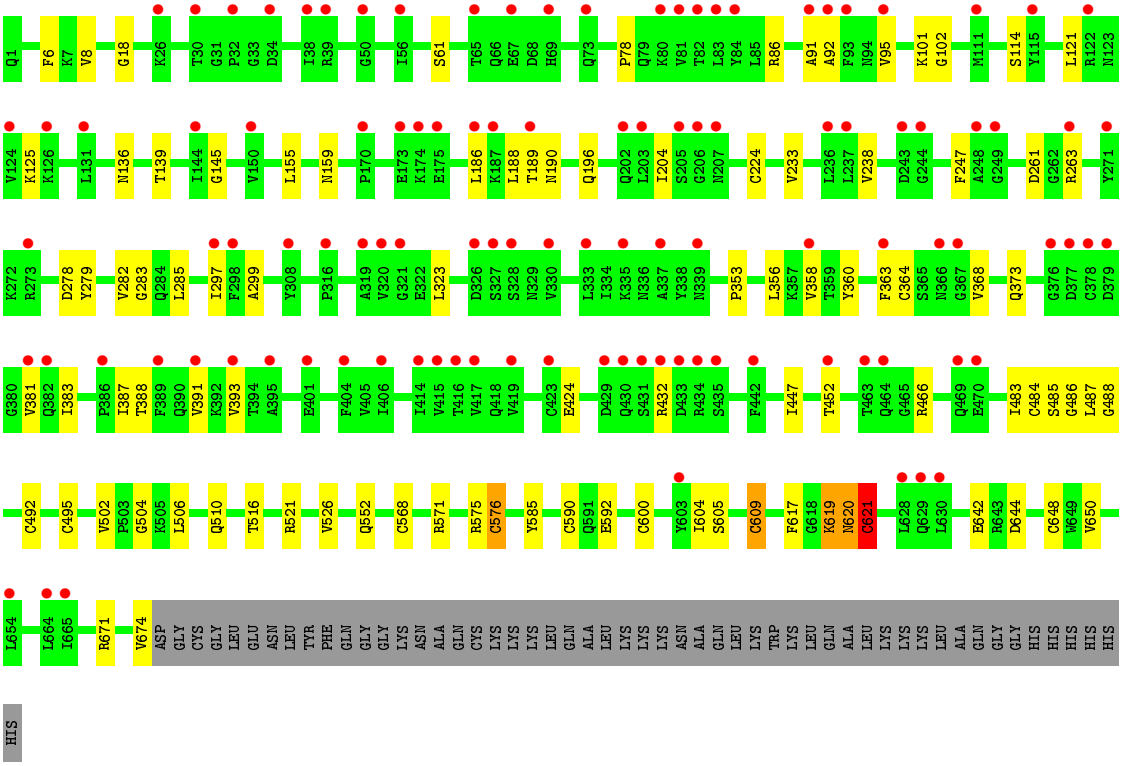
Chain F:





- 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

All (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
1	G	73	LEU	CA-CB-CG	6.19	129.54	115.30
1	E	73	LEU	CA-CB-CG	6.11	129.35	115.30
2	B	654	LEU	CA-CB-CG	6.08	129.29	115.30
2	H	609	CYS	CA-CB-SG	6.04	124.88	114.00
1	A	663	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	G	899	LEU	CA-CB-CG	5.46	127.86	115.30
1	C	73	LEU	CA-CB-CG	5.39	127.70	115.30
1	G	849	LEU	CA-CB-CG	5.23	127.32	115.30
1	C	752	CYS	CA-CB-SG	-5.13	104.76	114.00
1	E	86	LEU	CA-CB-CG	5.08	126.99	115.30
2	F	492	CYS	CA-CB-SG	-5.02	104.96	114.00

There are no chirality outliers.

All (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
2	B	231	ARG	Peptide
1	C	600	LEU	Peptide
1	C	601	TRP	Peptide
1	C	622	GLU	Peptide
1	C	690	LYS	Peptide
1	C	82	SER	Peptide
1	C	884	GLU	Peptide
2	D	102	GLY	Peptide
2	D	433	ASP	Peptide
2	D	436	LEU	Peptide
2	D	437	CYS	Peptide
2	D	620	ASN	Peptide
1	E	465	TYR	Peptide
1	E	640	ASP	Peptide
1	E	82	SER	Peptide
1	G	642	ARG	Peptide
1	G	729	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	G	82	SER	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
2:D:185:VAL:HG12	2:D:186:LEU:HG	1.70	0.72
1:A:688:GLY:HA3	1:E:632:GLN:OE1	1.89	0.72
1:E:622:GLU:OE1	1:G:960:GLN:NE2	2.23	0.72
1:G:823:ARG:HG3	1:G:859:PHE:HB2	1.70	0.72
1:G:642:ARG:HA	1:G:644:LYS:HG3	1.71	0.72
2:D:434:ARG:O	2:D:435:SER:HB3	1.91	0.71
1:G:438:TYR:HD1	1:G:441:ALA:HB2	1.56	0.71
1:C:659:ASP:HB2	1:C:716:ASN:HB2	1.71	0.70
1:E:659:ASP:HB2	1:E:716:ASN:OD1	1.91	0.70
1:A:434:GLN:HB3	1:A:437:SER:HB3	1.72	0.70
2:H:604:ILE:HD11	2:H:642:GLU:HB2	1.73	0.70
1:E:917:LYS:NZ	2:F:642:GLU:OE1	2.24	0.69
2:B:158:VAL:HG12	2:B:207:ASN:HA	1.72	0.69
1:C:407:ARG:NH2	2:D:245:PHE:O	2.25	0.69
1:E:93:VAL:HB	1:E:104:THR:O	1.93	0.69
5:G:3070:NAG:O7	5:G:3070:NAG:O3	2.09	0.69
1:G:716:ASN:HB3	1:G:741:TYR:CE1	2.28	0.69
1:A:173:GLN:HE22	1:A:202:GLN:HA	1.58	0.69
1:E:918:TYR:HE1	1:E:1079:GLU:HB3	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:757:ILE:O	1:E:758:CYS:HB2	1.92	0.68
1:A:161:GLN:HG2	1:A:311:LYS:HD3	1.75	0.68
1:C:739:GLN:HG3	1:C:741:TYR:H	1.58	0.68
1:E:12:ARG:NE	1:E:590:GLN:OE1	2.27	0.68
1:A:307:GLN:HG2	1:A:311:LYS:HE3	1.74	0.68
1:C:741:TYR:OH	5:C:3716:NAG:O5	2.11	0.68
1:E:481:GLY:HA2	1:E:1021:GLN:CB	2.23	0.68
1:A:406:PRO:HB3	1:A:438:TYR:CZ	2.30	0.67
6:G:3072:BMA:H5	7:G:3074:MAN:H3	1.76	0.67
2:B:184:HIS:NE2	2:B:186:LEU:O	2.27	0.67
1:C:748:PHE:O	1:C:885:ASN:ND2	2.24	0.67
2:D:76:LEU:HD21	2:D:97:PHE:HD1	1.60	0.67
1:A:479:PRO:HD3	1:A:485:TRP:CD1	2.29	0.67
2:D:104:PRO:HB3	2:D:139:THR:HB	1.76	0.67
1:C:601:TRP:HZ3	1:C:639:ILE:HG22	1.59	0.67
2:B:379:ASP:OD1	2:B:380:GLY:N	2.28	0.67
1:G:899:LEU:HD12	1:G:900:PRO:HD2	1.77	0.66
1:C:956:VAL:O	1:C:963:VAL:N	2.26	0.66
1:C:100:ASN:HB2	2:D:159:ASN:ND2	2.11	0.66
2:B:232:ASN:O	2:B:233:VAL:HG13	1.95	0.66
2:F:271:TYR:O	2:F:273:ARG:N	2.28	0.66
1:A:311:LYS:HB3	1:A:315:PHE:HE2	1.61	0.66
2:D:343:SER:HA	2:D:381:VAL:O	1.95	0.66
5:G:3071:NAG:O7	5:G:3071:NAG:O3	2.11	0.65
1:C:638:TYR:HB3	1:C:691:ALA:HB2	1.77	0.65
1:E:410:HIS:CD2	2:F:307:THR:HG21	2.31	0.65
1:A:528:GLU:O	1:A:531:ARG:HG2	1.96	0.65
1:A:71:MET:HB3	1:A:93:VAL:HG22	1.78	0.65
1:C:411:THR:HG22	1:C:435:ILE:HA	1.79	0.65
1:C:521:VAL:HG12	1:C:569:LEU:HD13	1.79	0.65
5:C:3920:NAG:H5	2:D:674:VAL:HG21	1.78	0.64
1:A:517:LEU:HD11	1:A:541:LEU:HD23	1.78	0.64
1:A:917:LYS:NZ	2:B:642:GLU:HB3	2.12	0.64
1:A:329:GLU:OE2	5:A:3374:NAG:H5	1.97	0.64
1:G:741:TYR:CD2	2:H:502:VAL:HG12	2.33	0.64
1:A:406:PRO:HB3	1:A:438:TYR:CE2	2.33	0.64
2:F:261:ASP:N	2:F:261:ASP:OD1	2.31	0.64
1:G:71:MET:HB3	1:G:93:VAL:HG22	1.80	0.64
1:E:354:PHE:HB3	5:E:3373:NAG:H83	1.80	0.64
1:A:929:SER:OG	5:A:3031:NAG:O7	2.15	0.63
2:H:605:SER:O	2:H:609:CYS:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:3375:BMA:O4	7:G:3376:MAN:H3	1.99	0.63
1:E:775:LEU:HB3	1:E:778:SER:HB3	1.79	0.63
1:A:139:GLY:HA3	1:A:173:GLN:HE21	1.62	0.63
1:E:451:ASP:OD2	8:E:4001:HOH:O	2.15	0.63
1:E:103:LEU:HD21	2:F:155:LEU:HD13	1.81	0.63
2:H:619:LYS:O	2:H:621:CYS:N	2.31	0.63
1:E:67:GLU:HG2	1:E:123:ARG:HD3	1.81	0.63
2:F:593:CYS:O	2:F:595:GLY:N	2.32	0.62
1:G:76:SER:HB3	1:G:89:CYS:HB2	1.80	0.62
1:A:436:GLY:HA3	2:B:282:VAL:HG21	1.79	0.62
1:A:1071:ARG:HH21	1:C:755:ASP:HB2	1.64	0.62
1:E:471:GLY:HA3	1:E:502:PHE:HB3	1.81	0.62
1:E:811[B]:ARG:NH1	8:E:4003:HOH:O	2.31	0.62
2:B:225:PRO:HA	2:B:229:GLY:H	1.63	0.62
1:E:407:ARG:O	1:E:410:HIS:N	2.30	0.62
1:A:605:SER:HB3	1:A:636:CYS:HB2	1.82	0.62
1:C:918:TYR:CE1	1:C:1079:GLU:HB3	2.35	0.62
1:C:791:ASP:HB2	8:C:4006:HOH:O	2.00	0.62
1:A:562:LEU:HD21	1:A:590:GLN:HE21	1.65	0.61
1:C:481:GLY:HA3	1:C:1022:GLU:HA	1.83	0.61
1:C:929:SER:OG	5:C:3031:NAG:O7	2.17	0.61
1:A:438:TYR:CD1	1:A:441:ALA:HB2	2.34	0.61
1:A:458:LEU:HD21	1:A:545:ILE:HD12	1.81	0.61
1:C:469:ARG:HH11	1:C:495:GLN:HG2	1.65	0.61
1:C:605:SER:HB3	1:C:636:CYS:HB2	1.83	0.61
1:E:562:LEU:HD21	1:E:590:GLN:NE2	2.16	0.61
2:D:231:ARG:HG2	2:D:231:ARG:HH11	1.65	0.60
1:E:1069:PHE:CE2	2:F:584:GLY:HA3	2.36	0.60
1:G:71:MET:HE2	1:G:73:LEU:HB3	1.83	0.60
1:A:24:GLN:HG2	1:A:575:LEU:HD11	1.84	0.60
5:A:3880:NAG:O3	5:A:3880:NAG:O7	2.16	0.60
1:E:501:ARG:NH1	8:E:4004:HOH:O	2.34	0.60
1:E:750:LYS:HE3	1:E:796:TYR:HB2	1.83	0.60
1:C:113:THR:O	1:E:931:VAL:HG21	2.01	0.60
1:G:9:THR:HB	1:G:593:LEU:HB3	1.84	0.60
2:B:323:LEU:HB2	2:B:329:ASN:OD1	2.02	0.60
1:C:601:TRP:HB3	1:C:642:ARG:HH21	1.65	0.60
1:C:925:GLU:N	1:C:925:GLU:OE1	2.35	0.60
1:E:781:GLU:HG2	1:E:811[B]:ARG:HH22	1.67	0.60
1:G:640:ASP:OD1	1:G:641:LYS:N	2.33	0.59
2:H:486:GLY:O	2:H:488:GLY:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:918:TYR:HE2	5:C:3920:NAG:O5	1.84	0.59
2:D:451:ASP:OD1	2:D:452:THR:N	2.33	0.59
2:B:184:HIS:HB3	2:B:269:ASN:HB3	1.84	0.59
2:D:324:SER:H	2:D:329:ASN:HD21	1.50	0.59
1:C:411:THR:O	8:C:4001:HOH:O	2.17	0.59
5:A:3070:NAG:O7	5:A:3070:NAG:O3	2.17	0.59
1:G:659:ASP:OD2	5:G:3716:NAG:N2	2.36	0.59
2:D:502:VAL:O	2:D:505:LYS:HB3	2.03	0.59
1:C:1032:LEU:HD21	1:C:1078:LEU:HD11	1.85	0.59
1:A:54:THR:HG22	1:A:56:ALA:H	1.67	0.58
1:E:354:PHE:CE1	5:E:3373:NAG:H4	2.37	0.58
1:C:601:TRP:CH2	1:C:643:SER:HA	2.37	0.58
1:G:880:ASN:ND2	5:G:3880:NAG:O7	2.36	0.58
1:G:909:VAL:HG23	1:G:938:VAL:HB	1.85	0.58
1:A:131:GLN:O	1:A:228:ARG:NH2	2.37	0.58
1:C:1043:LYS:O	1:C:1079:GLU:HA	2.03	0.58
1:E:538:HIS:CD2	1:E:550:SER:HG	2.21	0.58
1:E:436:GLY:HA3	2:F:282:VAL:HG21	1.86	0.58
1:A:575:LEU:N	1:A:582:ASP:OD2	2.37	0.58
2:B:174:LYS:HG3	2:B:175:GLU:H	1.68	0.58
1:C:43:GLN:O	5:C:3070:NAG:H82	2.03	0.58
1:E:87:LEU:HD21	1:E:348:LEU:HD21	1.86	0.58
1:A:789:TRP:CE2	1:C:772:LYS:HB3	2.39	0.58
1:C:866:SER:HB3	1:C:869:ALA:HB2	1.85	0.58
2:D:362:SER:OG	2:D:378:CYS:SG	2.61	0.58
2:D:462:GLN:H	2:D:462:GLN:NE2	2.02	0.58
1:E:766:PHE:HB3	1:E:786:VAL:HG22	1.86	0.58
1:E:833:PRO:HA	1:E:840:TRP:CD1	2.38	0.58
1:C:643:SER:O	1:C:645:ASN:N	2.36	0.57
1:A:701:PRO:HG2	1:A:704:VAL:HG22	1.84	0.57
1:C:12:ARG:HB2	1:C:590:GLN:HE21	1.69	0.57
1:G:946:LEU:HD21	1:G:1055:PHE:HD2	1.68	0.57
1:A:922:SER:OG	5:A:3920:NAG:H82	2.04	0.57
1:C:436:GLY:HA3	2:D:282:VAL:HG21	1.85	0.57
1:E:376:GLN:HB2	5:E:3373:NAG:H3	1.86	0.57
5:G:3042:NAG:H2	5:G:3070:NAG:C8	2.34	0.57
2:B:350:ASN:OD1	2:B:351:ALA:N	2.31	0.57
2:B:579:CYS:HB3	2:B:590:CYS:SG	2.45	0.57
2:D:231:ARG:HG2	2:D:231:ARG:NH1	2.19	0.57
2:F:305:VAL:HG21	2:F:322:GLU:HB2	1.86	0.57
2:F:486:GLY:O	2:F:488:GLY:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:768:PHE:HZ	1:E:877:LEU:HD21	1.70	0.57
2:H:101:LYS:HG3	2:H:383:ILE:HD13	1.86	0.57
1:A:804:HIS:CE1	1:A:840:TRP:HB2	2.40	0.57
1:A:689:LEU:HB2	1:E:609:ILE:HD13	1.86	0.57
1:A:897:LEU:HD13	1:C:897:LEU:HD13	1.85	0.57
1:E:509:LEU:HG	1:E:512:VAL:HG11	1.87	0.57
1:E:516:LYS:HE2	1:E:642:ARG:HH12	1.68	0.57
1:A:670:ARG:HH11	1:A:706:ASP:HB3	1.70	0.56
1:A:964:TRP:CD1	1:A:967:VAL:HG22	2.40	0.56
5:C:3373:NAG:O4	5:C:3374:NAG:O7	2.21	0.56
1:C:663:ASP:O	1:C:679:ARG:NH2	2.38	0.56
1:C:113:THR:HA	1:E:1031:ASN:OD1	2.05	0.56
2:F:61:SER:HB3	2:F:91:ALA:HB2	1.87	0.56
1:A:925:GLU:HG2	1:A:925:GLU:O	2.05	0.56
2:D:224:CYS:SG	2:D:266:LEU:HD11	2.45	0.56
1:E:642:ARG:O	1:E:643:SER:HB2	2.05	0.56
1:C:430:VAL:HG11	1:C:487:CYS:SG	2.45	0.56
1:C:630:LEU:HB2	1:G:725:LEU:HD11	1.86	0.56
2:B:155:LEU:HD12	2:B:156:PRO:HA	1.86	0.56
1:A:961:GLU:HG3	1:A:1039:GLN:CD	2.25	0.56
1:A:335:GLU:OE2	1:A:363:TYR:OH	2.24	0.56
1:A:486:TRP:HB2	2:B:588:PRO:HD3	1.87	0.56
1:A:659:ASP:CG	5:A:3716:NAG:H82	2.26	0.56
1:A:788:VAL:HG21	1:A:881:VAL:HG21	1.88	0.56
1:E:47:LEU:HB3	1:E:60:ILE:HD12	1.88	0.56
1:G:395[B]:TRP:O	1:G:397:GLY:N	2.38	0.56
1:G:455:ASP:HA	1:G:478:LEU:HD23	1.88	0.56
1:G:913:GLU:N	1:G:913:GLU:OE1	2.33	0.56
1:G:115:LEU:H	1:G:115:LEU:HD23	1.70	0.56
2:D:323:LEU:HG	2:D:327:SER:HA	1.85	0.56
1:E:326:SER:O	1:E:355:THR:HB	2.04	0.56
1:E:663:ASP:O	1:E:679:ARG:NH2	2.39	0.56
1:A:480:ARG:HG3	1:A:1021:GLN:HB2	1.88	0.56
1:A:19:GLY:O	1:A:567:GLN:NE2	2.38	0.56
1:E:811[B]:ARG:HH21	1:E:862:THR:HG21	1.71	0.56
1:G:34:ALA:O	1:G:36:GLN:N	2.39	0.56
1:A:411:THR:HG22	1:A:435:ILE:HA	1.88	0.56
5:E:3717:NAG:O3	5:E:3717:NAG:O7	2.20	0.56
1:E:920:ASN:OD1	5:E:3920:NAG:H82	2.06	0.56
1:C:407:ARG:HD2	2:D:247:PHE:CZ	2.41	0.55
1:G:939:ASN:HB3	1:G:1023:GLU:HG2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:848:HIS:CG	2:H:485:SER:HB3	2.40	0.55
1:G:100:ASN:HB2	2:H:159:ASN:HD21	1.70	0.55
2:B:381:VAL:HG21	2:B:387:ILE:HG21	1.88	0.55
1:C:823:ARG:HB3	1:C:859:PHE:HB2	1.87	0.55
1:E:1071[B]:ARG:HH22	1:G:755:ASP:C	2.09	0.55
1:E:716:ASN:HB3	1:E:741:TYR:CE1	2.42	0.55
1:A:600:LEU:HD23	1:A:639:ILE:HD11	1.88	0.55
1:C:329:GLU:HB2	1:C:331:GLU:OE2	2.06	0.55
1:C:718:THR:HB	1:C:740[B]:ARG:HH22	1.72	0.55
2:D:441:GLY:HA3	2:D:459:CYS:SG	2.47	0.55
1:E:430:VAL:HG11	1:E:487:CYS:SG	2.46	0.55
1:E:76:SER:HB3	1:E:89:CYS:HB2	1.89	0.55
2:D:343:SER:HG	2:D:380:GLY:H	1.51	0.55
1:E:921:PHE:CZ	1:E:1037:VAL:HG11	2.42	0.55
2:H:101:LYS:HG2	2:H:102:GLY:H	1.71	0.55
1:A:308:ASN:O	1:A:311:LYS:HB2	2.07	0.55
1:E:781:GLU:CG	1:E:811[B]:ARG:HH22	2.19	0.55
1:A:667:LEU:N	2:B:489:ASP:OD2	2.28	0.55
6:C:3375:BMA:O4	7:C:3378:MAN:H2	2.07	0.55
1:A:674:GLN:HE22	1:E:653:GLN:NE2	2.05	0.55
1:A:390:THR:HG22	1:A:403:LEU:HG	1.89	0.55
2:B:593:CYS:O	2:B:595:GLY:N	2.39	0.55
2:D:617:PHE:HA	2:D:620:ASN:HB2	1.89	0.55
1:C:811:ARG:HD2	2:D:520:GLU:OE2	2.07	0.55
1:C:923:GLU:O	1:C:926:GLU:HG3	2.07	0.55
1:E:342:THR:HG22	1:E:345:GLY:O	2.07	0.55
2:H:648:CYS:SG	2:H:671:ARG:NH2	2.80	0.55
2:B:346:PHE:HB2	2:B:409:LEU:HB2	1.89	0.54
1:E:406:PRO:HB3	1:E:438:TYR:CE1	2.42	0.54
2:F:295:GLN:HG3	2:F:317:LYS:HB3	1.87	0.54
2:D:324:SER:H	2:D:329:ASN:ND2	2.05	0.54
5:G:3920:NAG:O4	2:H:674:VAL:HG13	2.07	0.54
1:A:93:VAL:HB	1:A:104:THR:O	2.07	0.54
1:A:897:LEU:HD11	1:C:895:PHE:CZ	2.43	0.54
1:C:413:LYS:HG3	1:C:430:VAL:O	2.07	0.54
1:E:1044:LYS:NZ	1:E:1079:GLU:OE2	2.38	0.54
2:B:571:ARG:NH1	2:B:659:GLY:O	2.39	0.54
1:G:90:GLY:O	1:G:93:VAL:HG23	2.07	0.54
1:A:402:VAL:HG22	1:A:416:ILE:HG12	1.90	0.54
5:G:3042:NAG:H2	5:G:3070:NAG:H81	1.89	0.54
5:E:3070:NAG:O7	5:E:3070:NAG:O3	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ALA:O	1:C:43:GLN:HG2	2.07	0.54
1:E:866:SER:HB3	1:E:869:ALA:HB2	1.90	0.54
5:A:3716:NAG:H4	5:A:3717:NAG:HN2	1.73	0.54
2:D:108:TYR:HB3	2:D:237:LEU:HD23	1.89	0.54
1:A:918:TYR:H	1:A:1077:VAL:H	1.56	0.54
2:B:592:GLU:HG2	2:B:594:PRO:HD3	1.90	0.54
1:C:12:ARG:HD2	1:C:590:GLN:HE21	1.72	0.54
5:C:3042:NAG:O3	5:C:3042:NAG:O7	2.23	0.54
2:D:227:GLU:OE1	2:D:227:GLU:N	2.41	0.54
2:D:343:SER:OG	2:D:380:GLY:N	2.33	0.54
1:A:162:PHE:HB3	1:A:167:THR:HG21	1.90	0.53
1:E:916:THR:HG21	1:E:932:ALA:HA	1.90	0.53
1:E:963:VAL:HA	1:E:1036:TRP:CD1	2.42	0.53
1:A:795:SER:HB3	1:A:851:PHE:HB3	1.90	0.53
2:B:287:HIS:HE1	2:B:291:GLU:OE2	1.91	0.53
1:C:1029:LYS:HE3	1:E:113:THR:HB	1.89	0.53
1:C:354:PHE:CD2	5:C:3373:NAG:H2	2.44	0.53
1:C:805:PRO:HA	1:C:839:THR:HA	1.89	0.53
5:F:3094:NAG:O7	5:F:3094:NAG:O3	2.23	0.53
1:C:918:TYR:OH	1:C:1079:GLU:HB3	2.09	0.53
1:A:639:ILE:HG22	1:A:688:GLY:O	2.08	0.53
1:C:801:THR:HB	1:C:880:ASN:OD1	2.08	0.53
1:A:725:LEU:HD12	1:E:630:LEU:HB2	1.89	0.53
2:F:168:PRO:HB3	2:F:179:PRO:HG3	1.90	0.53
1:G:1062:GLN:HE21	1:G:1067:GLU:HA	1.73	0.53
1:G:642:ARG:HG2	1:G:644:LYS:HE3	1.90	0.53
5:A:3717:NAG:O3	5:A:3717:NAG:O7	2.25	0.53
1:A:624:VAL:O	1:A:625:VAL:HG12	2.08	0.53
1:C:615:ARG:HA	1:C:618:PHE:CE2	2.43	0.53
1:G:638:TYR:HB3	1:G:691:ALA:HA	1.91	0.53
2:H:585:TYR:HA	2:H:592:GLU:O	2.08	0.53
1:A:31:VAL:HG11	1:A:86:LEU:HD21	1.90	0.53
1:E:103:LEU:O	1:E:332:MET:HA	2.09	0.53
1:E:615:ARG:HA	1:E:618:PHE:CE1	2.44	0.53
1:G:385:TYR:CE2	1:G:407:ARG:HG3	2.44	0.53
5:A:3920:NAG:O3	5:A:3920:NAG:O7	2.21	0.53
1:E:921:PHE:HZ	1:E:1037:VAL:HG11	1.74	0.53
1:E:658:LEU:HD23	1:E:715:LEU:HD11	1.90	0.53
1:G:103:LEU:HD11	2:H:155:LEU:HD13	1.91	0.53
1:A:411:THR:OG1	1:A:412:GLY:N	2.42	0.53
2:D:19:PRO:HB3	2:D:89:GLN:NE2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:568:CYS:HB3	2:H:590:CYS:SG	2.49	0.53
2:B:353:PRO:HG2	2:B:402:GLN:NE2	2.23	0.52
2:D:184:HIS:NE2	2:D:266:LEU:HD22	2.24	0.52
2:D:469:GLN:C	2:D:471:LEU:H	2.12	0.52
1:E:759:GLN:O	1:E:793:GLU:N	2.23	0.52
2:F:460:GLU:HB3	8:F:4002:HOH:O	2.08	0.52
2:F:454:TYR:HA	2:F:462:GLN:HA	1.92	0.52
1:E:714:ARG:NH1	2:F:501:ASP:OD1	2.42	0.52
1:A:181:HIS:NE2	1:A:200:VAL:HG13	2.24	0.52
1:C:918:TYR:HE1	1:C:1079:GLU:HB3	1.72	0.52
1:C:889:ARG:HH21	1:C:892:LYS:HE2	1.75	0.52
2:D:383:ILE:O	2:D:385:VAL:HG23	2.09	0.52
1:G:716:ASN:ND2	5:G:3716:NAG:O7	2.43	0.52
1:G:385:TYR:CD2	1:G:407:ARG:HG3	2.45	0.52
1:G:407:ARG:HD2	2:H:247:PHE:CZ	2.45	0.52
1:G:655:SER:OG	1:G:720:VAL:O	2.27	0.52
1:A:917:LYS:HZ2	2:B:642:GLU:HB3	1.74	0.52
2:B:564:ARG:NH1	2:B:658:ASP:OD1	2.42	0.52
1:E:605:SER:HB3	1:E:636:CYS:HB2	1.91	0.52
1:G:918:TYR:H	1:G:1077:VAL:H	1.57	0.52
2:H:360:TYR:N	2:H:373:GLN:O	2.42	0.52
1:C:716:ASN:ND2	5:C:3716:NAG:O7	2.43	0.52
1:C:376:GLN:HB3	5:C:3373:NAG:H3	1.92	0.52
1:E:510:GLY:O	1:E:519:ASP:N	2.43	0.52
1:A:650:ARG:HD3	1:A:726:ALA:HB3	1.92	0.52
2:D:219:MET:HB2	2:D:285:LEU:HD21	1.90	0.52
1:E:388:TYR:CD2	1:E:406:PRO:HG2	2.45	0.52
1:E:800:ILE:O	1:E:844:CYS:N	2.39	0.52
1:G:929:SER:HB2	1:G:1031:ASN:HB3	1.91	0.52
1:G:757:ILE:O	1:G:758:CYS:HB2	2.10	0.52
1:C:444:CYS:HB2	1:C:506:LEU:HB2	1.91	0.52
2:D:350:ASN:HD22	2:D:405:VAL:HG22	1.75	0.52
1:E:103:LEU:HD12	2:F:156:PRO:HB3	1.92	0.52
1:A:137:ILE:HB	1:A:173:GLN:HA	1.91	0.52
1:C:931:VAL:HG22	1:C:1031:ASN:OD1	2.10	0.52
1:E:986:PRO:HD3	1:E:1007:GLY:HA2	1.91	0.52
1:E:759:GLN:HG3	1:E:793:GLU:HG2	1.91	0.52
1:A:47:LEU:HB3	1:A:60:ILE:HD12	1.92	0.52
1:G:951:ASN:HA	1:G:1011:PHE:O	2.10	0.52
1:G:436:GLY:HA3	2:H:282:VAL:HG21	1.92	0.52
1:G:9:THR:HG1	1:G:52:TYR:HD1	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:299:ALA:HB1	2:H:323:LEU:HD13	1.90	0.52
1:A:229:ARG:NH1	1:A:230:ASP:OD2	2.43	0.52
1:A:632:GLN:HG2	1:A:697:ASN:ND2	2.25	0.52
5:C:3071:NAG:O7	5:C:3071:NAG:H3	2.09	0.52
2:D:104:PRO:HG3	2:D:140:GLU:H	1.75	0.52
2:D:92:ALA:HA	2:D:391:VAL:O	2.10	0.52
1:G:905:VAL:HG11	1:G:946:LEU:HD22	1.91	0.52
2:H:617:PHE:HA	2:H:620:ASN:HB2	1.91	0.52
1:E:775:LEU:H	1:E:779:ASN:HD22	1.59	0.51
2:F:628:LEU:HD11	2:F:665:ILE:HB	1.91	0.51
1:G:412:GLY:HA3	1:G:439:PHE:HB3	1.92	0.51
1:A:12:ARG:HB3	1:A:590:GLN:OE1	2.10	0.51
1:C:836:SER:HB3	7:G:3884:MAN:O2	2.10	0.51
1:A:479:PRO:HG3	1:A:485:TRP:HB2	1.92	0.51
1:A:823:ARG:HG3	1:A:859:PHE:HB2	1.91	0.51
1:E:1052:GLU:CD	1:E:1071[B]:ARG:NH1	2.64	0.51
1:C:479:PRO:HG3	1:C:485:TRP:HB2	1.91	0.51
2:F:92:ALA:HA	2:F:391:VAL:O	2.11	0.51
1:A:69:VAL:HG12	1:A:70:ASN:OD1	2.11	0.51
2:D:299:ALA:HB1	2:D:323:LEU:HD13	1.92	0.51
2:D:436:LEU:O	2:D:437:CYS:HB2	2.10	0.51
5:E:3717:NAG:O3	6:E:3718:BMA:O5	2.27	0.51
1:E:790:ASN:HB2	1:E:851:PHE:CE2	2.45	0.51
1:E:851:PHE:HE1	1:E:857:ILE:HG12	1.76	0.51
2:D:617:PHE:HA	2:D:620:ASN:OD1	2.11	0.51
1:E:105:GLY:HA3	1:E:335:GLU:O	2.11	0.51
1:E:628:GLN:HG2	1:E:701:PRO:HA	1.92	0.51
1:A:93:VAL:O	1:A:103:LEU:HA	2.10	0.51
2:B:157:PHE:HA	2:B:209:ASP:HB2	1.92	0.51
1:E:917:LYS:NZ	2:F:642:GLU:HB2	2.26	0.51
1:A:480:ARG:HG3	1:A:1021:GLN:HG3	1.92	0.51
1:A:76:SER:HB3	1:A:89:CYS:HB2	1.93	0.51
1:E:651:ASP:OD1	1:E:652:LEU:N	2.43	0.51
1:E:705:GLU:OE1	1:E:705:GLU:N	2.44	0.51
1:C:918:TYR:H	1:C:1077:VAL:H	1.58	0.51
1:A:897:LEU:HD11	1:C:895:PHE:CE1	2.46	0.51
2:D:183:ARG:HG2	2:D:202:GLN:HE22	1.76	0.51
1:E:335:GLU:OE2	1:E:363:TYR:OH	2.18	0.51
1:E:649:SER:HA	1:E:652:LEU:HD12	1.92	0.51
2:H:364:CYS:HB3	2:H:368:VAL:HB	1.92	0.51
1:A:665:GLY:HA3	2:B:499:THR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:923:GLU:OE2	1:G:1038:ARG:NH2	2.35	0.50
5:C:3880:NAG:H3	5:C:3880:NAG:H83	1.92	0.50
1:E:939:ASN:HB3	1:E:1023:GLU:HB2	1.93	0.50
2:H:484:CYS:O	2:H:485:SER:HB2	2.10	0.50
2:D:155:LEU:HD12	2:D:156:PRO:HA	1.93	0.50
1:E:674:GLN:HB2	1:E:699:LEU:HG	1.93	0.50
1:E:880:ASN:HB3	1:E:894:THR:HG22	1.93	0.50
1:E:1069:PHE:HE2	2:F:584:GLY:HA3	1.77	0.50
1:G:866:SER:HB3	1:G:869:ALA:HB2	1.93	0.50
2:D:460:GLU:OE1	2:D:460:GLU:N	2.45	0.50
1:C:601:TRP:HB3	1:C:642:ARG:NH2	2.26	0.50
1:E:918:TYR:CE1	1:E:1079:GLU:HB3	2.43	0.50
1:E:897:LEU:HD11	1:G:895:PHE:CZ	2.47	0.50
2:B:554:GLU:OE1	2:B:577:ASN:ND2	2.44	0.50
2:B:6:PHE:O	2:B:8:VAL:HG23	2.12	0.50
1:C:476:CYS:HA	1:C:487:CYS:HA	1.93	0.50
1:G:563:GLN:HG3	1:G:588:ARG:HB3	1.92	0.50
1:C:692:HIS:CD2	1:G:694:GLU:HA	2.47	0.50
2:F:468:SER:O	2:F:472:GLU:HG3	2.11	0.50
1:G:1:PHE:HA	1:G:551:GLN:HG2	1.93	0.50
2:B:104:PRO:HB2	2:B:233:VAL:HG11	1.94	0.50
2:B:598:SER:OG	2:B:638:ARG:NE	2.45	0.50
1:A:786:VAL:HB	1:A:859:PHE:CE1	2.47	0.50
2:D:356:LEU:HD11	2:D:393:VAL:HG13	1.94	0.50
1:A:630:LEU:HD22	1:E:653:GLN:HB2	1.93	0.50
2:F:309:GLU:HA	2:F:320:VAL:HG11	1.94	0.50
2:B:240:ALA:HA	2:B:299:ALA:O	2.12	0.49
1:C:970:SER:HB3	1:C:1027:THR:OG1	2.11	0.49
1:C:1062:GLN:HE21	1:C:1067:GLU:HA	1.77	0.49
1:C:921:PHE:HE2	1:C:1037:VAL:HG21	1.77	0.49
2:D:183:ARG:HG2	2:D:202:GLN:OE1	2.12	0.49
2:D:469:GLN:O	2:D:471:LEU:N	2.43	0.49
1:E:972:PRO:O	1:E:975:PRO:HD3	2.12	0.49
1:G:47:LEU:HB3	1:G:60:ILE:HD12	1.94	0.49
2:B:564:ARG:HH21	2:B:657:GLN:NE2	2.10	0.49
1:C:919:LEU:HB2	1:C:930:HIS:CE1	2.46	0.49
1:E:747:PRO:HB3	1:E:884:GLU:HG2	1.93	0.49
7:G:3379:MAN:H62	7:G:3380:MAN:H3	1.94	0.49
1:A:1020:VAL:O	1:A:1022:GLU:N	2.44	0.49
1:A:340:VAL:HG21	1:A:391:GLU:HA	1.95	0.49
2:B:174:LYS:CG	2:B:175:GLU:H	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:618:GLY:C	2:B:620:ASN:H	2.15	0.49
1:C:38:ILE:HG23	5:C:3070:NAG:H81	1.95	0.49
1:C:601:TRP:N	1:C:601:TRP:CD2	2.80	0.49
2:D:468:SER:OG	2:D:469:GLN:O	2.23	0.49
2:B:108:TYR:HB3	2:B:237:LEU:HD23	1.94	0.49
1:E:1017:SER:O	1:E:1019:SER:N	2.45	0.49
6:G:3375:BMA:O2	7:G:3380:MAN:O6	2.11	0.49
2:H:278:ASP:OD1	2:H:279:TYR:N	2.45	0.49
2:D:105:ILE:HD11	2:D:236:LEU:HD12	1.95	0.49
1:E:768:PHE:CZ	1:E:877:LEU:HD21	2.48	0.49
5:G:3881:NAG:H83	5:G:3881:NAG:H3	1.94	0.49
1:A:238:ILE:HG12	1:A:267:ILE:HD12	1.95	0.49
1:A:919:LEU:HA	1:A:919:LEU:HD12	1.62	0.49
2:B:174:LYS:O	2:B:175:GLU:HB2	2.12	0.49
1:E:104:THR:HG21	1:E:124:GLN:HB2	1.94	0.49
1:E:35:PRO:O	1:E:72:SER:HA	2.12	0.49
1:G:609:ILE:HB	1:G:632:GLN:HB2	1.93	0.49
1:G:823:ARG:HB2	1:G:860:LEU:H	1.77	0.49
2:D:104:PRO:CB	2:D:139:THR:HB	2.42	0.49
1:A:47:LEU:HG	1:A:73:LEU:HD13	1.95	0.49
1:C:427:LYS:HE3	1:C:480:ARG:HH21	1.78	0.49
2:D:592:GLU:OE2	2:D:594:PRO:HB3	2.12	0.49
1:E:70:ASN:HB3	1:E:94:HIS:CE1	2.47	0.49
1:G:848:HIS:CD2	2:H:485:SER:HB3	2.48	0.49
1:A:347:VAL:HG21	1:A:401:LEU:HD21	1.95	0.49
1:A:953:TRP:HB3	1:A:1003:CYS:SG	2.53	0.49
1:E:539:GLY:HA2	1:E:545:ILE:HD13	1.93	0.49
2:F:323:LEU:HB3	2:F:333:LEU:HD11	1.95	0.49
1:G:536:LEU:HB3	1:G:551:GLN:HB2	1.95	0.49
1:G:663:ASP:O	1:G:679:ARG:NH2	2.45	0.49
1:G:946:LEU:HD21	1:G:1055:PHE:CD2	2.48	0.49
1:A:351:VAL:HG11	2:B:253:LEU:HD21	1.95	0.48
1:A:494:GLU:O	1:A:494:GLU:HG3	2.12	0.48
1:A:601:TRP:CD1	1:A:642:ARG:HB2	2.48	0.48
1:A:644:LYS:HA	1:A:644:LYS:HD3	1.61	0.48
1:A:714:ARG:NH1	1:A:741:TYR:CE1	2.81	0.48
1:C:515:ASP:O	1:C:516:LYS:HG2	2.13	0.48
2:D:18:GLY:O	2:D:86:ARG:NH2	2.46	0.48
1:E:516:LYS:HE2	1:E:642:ARG:NH1	2.28	0.48
1:A:9:THR:OG1	1:A:593:LEU:HB2	2.13	0.48
1:E:67:GLU:HG2	1:E:123:ARG:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:981:SER:HB3	1:E:1009:LEU:HD11	1.94	0.48
1:E:998:ASN:O	1:E:998:ASN:OD1	2.31	0.48
2:F:364:CYS:HB3	2:F:368:VAL:HB	1.93	0.48
1:G:395[A]:TRP:O	1:G:397:GLY:N	2.46	0.48
2:B:571:ARG:HA	2:B:582[B]:HIS:CE1	2.48	0.48
1:C:87:LEU:HD23	1:C:339:ALA:HB1	1.94	0.48
1:G:920:ASN:C	1:G:920:ASN:OD1	2.51	0.48
5:A:3070:NAG:O3	5:A:3071:NAG:O5	2.30	0.48
2:B:158:VAL:HA	2:B:208:LEU:HB3	1.94	0.48
2:B:484:CYS:SG	8:B:4002:HOH:O	2.61	0.48
2:B:642:GLU:OE2	2:B:652:TYR:OH	2.25	0.48
2:D:97:PHE:O	2:D:386:PRO:HA	2.12	0.48
1:A:630:LEU:CD2	1:E:653:GLN:HB2	2.44	0.48
1:E:67:GLU:N	1:E:67:GLU:OE1	2.37	0.48
2:F:184:HIS:NE2	2:F:186:LEU:O	2.46	0.48
2:F:344:ARG:HD3	2:F:379:ASP:HB3	1.94	0.48
2:B:220:GLN:OE1	2:B:264:CYS:HA	2.13	0.48
2:D:183:ARG:HG2	2:D:202:GLN:NE2	2.28	0.48
2:F:617:PHE:HA	2:F:620:ASN:HB2	1.94	0.48
2:H:145:GLY:HA3	2:H:188:LEU:HD23	1.94	0.48
2:H:18:GLY:O	2:H:86:ARG:NH2	2.46	0.48
1:A:42:ASN:HA	5:A:3070:NAG:C5	2.44	0.48
1:E:438:TYR:HD1	1:E:441:ALA:HB2	1.79	0.48
1:G:953:TRP:HB3	1:G:1003:CYS:SG	2.54	0.48
1:A:618:PHE:CE1	1:A:707:SER:HB3	2.49	0.48
2:D:100:ALA:O	2:D:101:LYS:HB3	2.14	0.48
2:D:620:ASN:HB3	2:D:624:ALA:HB2	1.96	0.48
1:G:656:VAL:HG11	1:G:687:LEU:HG	1.95	0.48
1:A:134:VAL:HG22	1:A:170:SER:HB3	1.95	0.48
1:A:929:SER:HB2	1:A:1031:ASN:HB3	1.95	0.48
1:G:465:TYR:CG	2:H:283:GLY:HA3	2.49	0.48
2:H:388:THR:HG21	5:H:3094:NAG:H61	1.95	0.48
1:A:598:PRO:HB3	1:A:646:LEU:HD11	1.96	0.48
1:A:319:GLY:HA3	7:A:3381:MAN:O3	2.14	0.47
1:A:469:ARG:HD3	1:A:495:GLN:HB3	1.96	0.47
1:A:918:TYR:HA	1:A:1077:VAL:O	2.14	0.47
1:A:921:PHE:O	1:A:922:SER:OG	2.26	0.47
1:G:430:VAL:HG11	1:G:487:CYS:SG	2.54	0.47
2:H:114:SER:O	2:H:204:ILE:HD11	2.14	0.47
2:H:261:ASP:OD1	2:H:263:ARG:HB2	2.13	0.47
2:D:158:VAL:HG12	2:D:207:ASN:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:533:GLY:HA3	2:F:551:CYS:SG	2.54	0.47
2:H:136:ASN:HA	2:H:139:THR:O	2.14	0.47
1:A:352:GLY:HA2	1:A:356:TRP:HA	1.97	0.47
2:D:438:HIS:O	2:D:438:HIS:CD2	2.67	0.47
2:F:614:LYS:NZ	2:F:645:SER:OG	2.48	0.47
2:F:571:ARG:NH1	2:F:659:GLY:O	2.47	0.47
2:B:76:LEU:HD23	2:B:413:ASP:HB3	1.97	0.47
1:C:30:VAL:CG1	1:C:50:CYS:HB2	2.44	0.47
1:C:919:LEU:HD13	1:C:930:HIS:CG	2.49	0.47
2:D:355:THR:HG22	2:D:544:PRO:HG2	1.96	0.47
2:D:76:LEU:HD21	2:D:97:PHE:CD1	2.45	0.47
1:G:103:LEU:H	1:G:332:MET:HG2	1.79	0.47
2:D:447:ILE:HG12	2:D:448:CYS:O	2.14	0.47
1:A:387:GLY:HA2	1:A:403:LEU:HD23	1.95	0.47
1:A:925:GLU:HB2	1:A:928:GLU:HG3	1.97	0.47
2:B:216:ASP:HB3	2:B:271:TYR:CE2	2.49	0.47
2:D:186:LEU:HD21	2:D:198:GLU:HB2	1.97	0.47
2:D:235:ARG:O	2:D:236:LEU:HD23	2.15	0.47
1:E:1045:VAL:HG13	1:E:1078:LEU:HB2	1.95	0.47
1:E:879:ALA:O	1:E:894:THR:HA	2.15	0.47
1:E:876:LEU:HD13	1:E:898:GLU:HB2	1.97	0.47
2:F:461:CYS:SG	8:F:4002:HOH:O	2.61	0.47
2:B:149:PHE:HA	2:B:181:ALA:O	2.15	0.47
1:C:1042:GLN:HG3	1:C:1044:LYS:H	1.80	0.47
2:D:500:SER:O	2:D:505:LYS:HB2	2.14	0.47
1:G:80:THR:HG22	1:G:85:GLN:HB2	1.97	0.47
1:G:100:ASN:HB2	2:H:159:ASN:ND2	2.29	0.47
1:A:609:ILE:HB	1:A:632:GLN:HB2	1.96	0.47
2:D:232:ASN:HB2	5:D:3232:NAG:H2	1.96	0.47
1:E:917:LYS:HZ3	2:F:642:GLU:HB2	1.80	0.47
1:E:757:ILE:HG12	1:G:1054:THR:HG21	1.97	0.47
2:H:424:GLU:H	2:H:424:GLU:CD	2.18	0.47
2:B:287:HIS:CE1	2:B:291:GLU:OE2	2.67	0.47
1:C:86:LEU:O	1:C:109:LEU:HD12	2.15	0.47
1:C:1069:PHE:CE2	2:D:584:GLY:HA3	2.50	0.47
1:E:998:ASN:O	1:E:1000:VAL:N	2.46	0.47
2:F:215:LEU:HB3	2:F:280:PRO:HG2	1.95	0.47
1:G:438:TYR:CD1	1:G:441:ALA:HB2	2.43	0.47
1:A:660:LEU:HB3	1:A:713:LEU:HD11	1.96	0.47
1:A:958:LEU:HG	1:A:959:ASN:OD1	2.15	0.47
2:B:278:ASP:OD1	2:B:279:TYR:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:GLN:HG3	2:B:317:LYS:HB3	1.97	0.47
1:A:757:ILE:HG21	1:C:1054:THR:HG21	1.96	0.47
2:D:220:GLN:O	2:D:224:CYS:SG	2.73	0.47
2:D:350:ASN:ND2	2:D:405:VAL:H	2.13	0.47
2:D:504:GLY:O	2:D:516:THR:OG1	2.32	0.47
2:F:219:MET:HA	2:F:285:LEU:HD21	1.97	0.47
1:G:381:MET:SD	1:G:413:LYS:NZ	2.78	0.47
1:A:385:TYR:HB3	1:A:388:TYR:HB2	1.96	0.47
1:C:887:THR:OG1	8:C:4002:HOH:O	2.20	0.47
2:F:300:VAL:HG11	2:F:308:TYR:CE2	2.50	0.47
5:C:3374:NAG:O3	6:C:3375:BMA:H2	2.15	0.46
1:C:437:SER:O	1:C:461:ALA:HB1	2.14	0.46
1:C:469:ARG:HB3	1:C:495:GLN:HA	1.97	0.46
2:D:115:TYR:CD1	2:D:170:PRO:HD2	2.50	0.46
1:E:808:LEU:HA	1:E:864:ASP:O	2.15	0.46
5:G:3070:NAG:HO3	5:G:3070:NAG:C7	2.21	0.46
1:G:411:THR:HG22	1:G:435:ILE:HA	1.96	0.46
1:A:1020:VAL:C	1:A:1022:GLU:H	2.18	0.46
1:A:961:GLU:HG3	1:A:1039:GLN:NE2	2.30	0.46
1:C:17:GLY:HA2	1:C:588:ARG:NH1	2.30	0.46
2:F:36[B]:ASP:OD1	2:F:37:SER:N	2.46	0.46
1:G:717:PHE:HA	5:G:3716:NAG:H81	1.96	0.46
1:G:892:LYS:NZ	5:G:3880:NAG:H2	2.30	0.46
1:C:951:ASN:HA	1:C:1011:PHE:O	2.15	0.46
2:D:115:TYR:CE1	2:D:170:PRO:HD2	2.51	0.46
2:D:316:PRO:HB3	2:D:375:ARG:NH2	2.30	0.46
1:G:93:VAL:HB	1:G:104:THR:O	2.15	0.46
6:G:3375:BMA:O4	7:G:3376:MAN:H5	2.15	0.46
2:H:552:GLN:O	8:H:4001:HOH:O	2.20	0.46
1:A:399:GLN:N	1:A:399:GLN:OE1	2.45	0.46
1:A:87:LEU:HD12	1:A:109:LEU:HD13	1.97	0.46
1:C:659:ASP:OD2	5:C:3716:NAG:H82	2.15	0.46
1:C:47:LEU:HB3	1:C:60:ILE:HD12	1.96	0.46
1:C:657:THR:O	1:C:717:PHE:HA	2.16	0.46
1:G:1067:GLU:O	1:G:1070:MET:HG2	2.15	0.46
1:G:43:GLN:OE1	1:G:43:GLN:HA	2.15	0.46
1:A:1057:THR:HB	1:C:761:ASN:HD22	1.81	0.46
1:A:185:GLU:OE2	1:A:189:ARG:NH2	2.38	0.46
1:E:407:ARG:NH2	2:F:247:PHE:H	2.14	0.46
1:G:12:ARG:HA	1:G:590:GLN:HB3	1.98	0.46
1:G:747:PRO:HB3	1:G:884:GLU:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:353:PRO:HD2	2:H:356:LEU:HD21	1.97	0.46
1:A:908:VAL:HG12	1:A:1069:PHE:HB3	1.96	0.46
1:A:980:SER:O	1:A:1011:PHE:HA	2.15	0.46
2:B:212:GLU:OE2	2:B:241:THR:HG21	2.15	0.46
1:C:1069:PHE:HE2	2:D:584:GLY:HA3	1.78	0.46
1:C:469:ARG:HD3	1:C:495:GLN:HG2	1.97	0.46
1:C:469:ARG:NH1	1:C:495:GLN:OE1	2.49	0.46
1:C:520:VAL:O	1:C:536:LEU:HD12	2.16	0.46
1:E:364:PRO:HB2	1:E:367:MET:HG3	1.98	0.46
1:E:715:LEU:N	1:E:742:PHE:O	2.47	0.46
1:E:613:ILE:O	1:E:749:GLU:HB2	2.16	0.46
5:G:3071:NAG:C7	5:G:3071:NAG:HO3	2.23	0.46
1:A:376:GLN:O	1:A:376:GLN:HG2	2.16	0.46
1:E:874:ARG:HH21	1:E:898:GLU:HG2	1.81	0.46
1:G:683:ARG:CZ	1:G:685:ARG:HH22	2.29	0.46
1:A:789:TRP:CZ2	1:C:772:LYS:HB3	2.51	0.46
1:A:915:PHE:CE2	1:A:917:LYS:HB3	2.51	0.46
2:B:605:SER:O	2:B:609:CYS:HB2	2.16	0.46
1:C:521:VAL:HG11	1:C:583:LEU:HD21	1.98	0.46
2:D:350:ASN:ND2	2:D:405:VAL:HG22	2.31	0.46
2:F:611:LYS:HE2	2:F:669:GLU:HG2	1.96	0.46
2:H:521:ARG:HG2	2:H:526:VAL:HA	1.98	0.46
1:A:633:SER:HB2	1:A:698:LEU:HD11	1.98	0.46
1:A:91:PRO:HG3	1:A:337:PHE:HA	1.98	0.46
2:D:129:GLY:HA3	2:D:133:ARG:HH12	1.80	0.46
2:D:300:VAL:HG11	2:D:308:TYR:CE2	2.51	0.46
1:E:716:ASN:HB3	1:E:741:TYR:CD1	2.51	0.46
2:F:240:ALA:HA	2:F:299:ALA:O	2.15	0.46
1:E:410:HIS:HD2	2:F:307:THR:HG21	1.79	0.46
1:G:608:PHE:CE2	1:G:746:LEU:HB2	2.51	0.46
1:A:510:GLY:O	1:A:519:ASP:N	2.42	0.45
1:A:805:PRO:HA	1:A:839:THR:HA	1.98	0.45
1:C:918:TYR:OH	5:C:3920:NAG:H4	2.16	0.45
2:D:617:PHE:CA	2:D:620:ASN:HB2	2.45	0.45
2:D:6:PHE:CD2	2:D:7:LYS:N	2.83	0.45
1:E:790:ASN:HB3	1:E:853:GLY:O	2.16	0.45
1:G:104:THR:HG22	1:G:105:GLY:H	1.81	0.45
1:A:802:PHE:O	1:A:841:SER:HA	2.17	0.45
1:A:438:TYR:OH	2:B:249:GLY:O	2.34	0.45
2:D:227:GLU:HG2	2:D:266:LEU:HD13	1.97	0.45
1:E:642:ARG:HG3	1:E:644:LYS:NZ	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:3718:BMA:O4	7:G:3719:MAN:H3	2.16	0.45
2:H:121:LEU:HD11	2:H:125:LYS:HE3	1.97	0.45
1:E:610:PRO:HD2	1:E:631:VAL:HG13	1.98	0.45
1:E:637:LEU:HD11	1:E:658:LEU:HD21	1.99	0.45
1:G:670:ARG:NH2	1:G:710:PRO:O	2.49	0.45
2:B:184:HIS:NE2	2:B:228:ILE:HG12	2.31	0.45
1:C:405:ALA:O	1:C:412:GLY:HA2	2.16	0.45
1:C:521:VAL:HG21	1:C:583:LEU:HD22	1.98	0.45
1:G:475:VAL:O	1:G:488:ASP:N	2.48	0.45
1:A:164:ARG:HB2	1:A:165:PRO:HA	1.98	0.45
1:A:909:VAL:HG23	1:A:938:VAL:HB	1.98	0.45
1:C:434:GLN:O	1:C:437:SER:HB3	2.16	0.45
1:C:480:ARG:C	1:C:480:ARG:HD3	2.36	0.45
1:C:650:ARG:C	1:C:652:LEU:H	2.20	0.45
1:C:934:HIS:HE2	1:C:1076:THR:HB	1.82	0.45
2:D:573:ARG:HD2	2:D:575:ARG:NH2	2.31	0.45
1:E:564:TYR:HB2	1:E:588:ARG:HB2	1.98	0.45
1:E:851:PHE:CE1	1:E:857:ILE:HG12	2.51	0.45
2:F:572:GLY:HA2	2:F:581:CYS:HA	1.99	0.45
1:G:384:SER:HB2	1:G:405:ALA:HB1	1.98	0.45
1:A:389:SER:O	1:A:403:LEU:HA	2.15	0.45
1:E:448:VAL:HA	1:E:518:THR:HB	1.99	0.45
1:G:532:GLY:HA3	1:G:565:PHE:HB3	1.97	0.45
1:A:940:ASN:CG	1:A:1020:VAL:HA	2.37	0.45
2:B:189:THR:OG1	2:B:190:ASN:N	2.50	0.45
2:D:309:GLU:HA	2:D:320:VAL:HG21	1.98	0.45
2:D:5:LYS:HD2	2:D:37:SER:HB2	1.98	0.45
1:G:115:LEU:HG	1:G:117:GLN:NE2	2.31	0.45
1:G:921:PHE:CZ	1:G:1080:LYS:HA	2.52	0.45
1:A:494:GLU:OE2	1:A:552:ARG:CZ	2.65	0.45
1:C:1043:LYS:HG2	1:C:1080:LYS:HD3	1.98	0.45
1:C:804:HIS:O	1:C:840:TRP:N	2.46	0.45
1:C:919:LEU:HD22	1:C:930:HIS:CD2	2.52	0.45
2:D:108:TYR:HB3	2:D:237:LEU:CD2	2.47	0.45
1:E:445:SER:HB2	1:E:454:THR:HG21	1.98	0.45
1:E:638:TYR:HB3	1:E:691:ALA:HB2	1.98	0.45
1:E:93:VAL:O	1:E:103:LEU:HA	2.16	0.45
1:A:638:TYR:HB3	1:A:691:ALA:HB2	1.99	0.45
1:C:918:TYR:CE2	5:C:3920:NAG:O5	2.68	0.45
1:G:67:GLU:HB3	1:G:123:ARG:HD3	1.99	0.45
1:G:729:ASN:HD22	1:G:729:ASN:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:921:PHE:CE2	1:C:1037:VAL:HG21	2.52	0.45
2:D:231:ARG:O	2:D:233:VAL:N	2.48	0.45
2:D:76:LEU:HD12	2:D:413:ASP:OD2	2.17	0.45
1:E:407:ARG:O	1:E:408:TYR:C	2.56	0.45
1:A:951:ASN:HA	1:A:1011:PHE:O	2.17	0.44
1:A:940:ASN:ND2	1:A:1018:PHE:O	2.43	0.44
1:A:80:THR:HG22	1:A:85:GLN:HB2	1.99	0.44
2:B:143:ARG:NH1	2:B:231:ARG:HD3	2.32	0.44
1:C:597:ARG:NH2	1:C:733:MET:SD	2.90	0.44
1:E:411:THR:HG22	1:E:435:ILE:HA	1.99	0.44
1:A:926:GLU:OE2	1:A:1038:ARG:NH2	2.46	0.44
1:A:512:VAL:HB	1:A:519:ASP:OD2	2.16	0.44
1:C:796:TYR:O	1:C:884:GLU:HG3	2.18	0.44
1:E:352:GLY:HA2	1:E:356:TRP:HA	2.00	0.44
1:E:604:VAL:HG21	1:E:742:PHE:CD2	2.52	0.44
1:G:94:HIS:NE2	2:H:155:LEU:HD11	2.32	0.44
2:D:356:LEU:HD11	2:D:393:VAL:CG1	2.47	0.44
2:F:270:LEU:HG	2:F:271:TYR:H	1.82	0.44
1:G:575:LEU:HD12	1:G:593:LEU:HD11	2.00	0.44
1:G:946:LEU:HD13	1:G:1060:TYR:CD2	2.52	0.44
1:A:643:SER:OG	1:A:644:LYS:N	2.50	0.44
1:A:876:LEU:HD11	1:A:896:GLN:HB2	2.00	0.44
1:C:394:LEU:HD22	1:C:395:TRP:H	1.82	0.44
1:C:903:TYR:HD2	1:C:944[B]:ARG:HH12	1.66	0.44
1:C:986:PRO:HG3	1:C:1005:ILE:O	2.18	0.44
1:E:937:GLN:NE2	1:E:1023:GLU:OE1	2.49	0.44
1:E:830:ASP:N	1:E:830:ASP:OD1	2.50	0.44
1:E:351:VAL:HG11	2:F:253:LEU:HD21	2.00	0.44
1:G:618:PHE:CZ	1:G:707:SER:HB3	2.53	0.44
1:C:953:TRP:HB3	1:C:1003:CYS:SG	2.58	0.44
2:D:237:LEU:O	2:D:296:PRO:HA	2.18	0.44
1:G:30:VAL:HB	1:G:50:CYS:HB2	1.99	0.44
1:G:611:ALA:O	1:G:747:PRO:HD2	2.17	0.44
1:A:12:ARG:HB3	1:A:590:GLN:HB3	1.98	0.44
1:C:1053:ILE:HB	1:C:1070:MET:HB2	2.00	0.44
1:E:80:THR:HG22	1:E:85:GLN:HB2	1.99	0.44
1:E:880:ASN:OD1	1:E:880:ASN:O	2.36	0.44
1:G:459:ILE:HD11	1:G:485:TRP:CZ2	2.53	0.44
1:G:803:SER:HB3	1:G:878:THR:OG1	2.17	0.44
1:A:483:ARG:HH22	1:A:939:ASN:ND2	2.16	0.44
1:C:76:SER:HB3	1:C:89:CYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:242:ASP:O	2:D:303:ARG:NH2	2.48	0.44
1:E:37:LYS:O	1:E:45:GLY:N	2.46	0.44
1:E:918:TYR:HA	1:E:1077:VAL:O	2.17	0.44
2:F:15:ILE:HG23	2:F:86:ARG:CZ	2.47	0.44
2:F:76:LEU:HD23	2:F:413:ASP:HB3	2.00	0.44
1:C:394:LEU:HD23	1:C:394:LEU:HA	1.59	0.44
2:F:506:LEU:HD23	2:F:506:LEU:HA	1.78	0.44
6:G:3882:BMA:H2	7:G:3883:MAN:H5	2.00	0.44
1:G:920:ASN:HB2	5:G:3920:NAG:O7	2.17	0.44
2:H:504:GLY:O	2:H:516:THR:OG1	2.25	0.44
1:A:181:HIS:CD2	1:A:200:VAL:HG22	2.53	0.43
1:A:632:GLN:HE21	1:A:697:ASN:HD21	1.66	0.43
2:B:301:THR:HG22	2:B:303:ARG:H	1.83	0.43
1:C:905:VAL:HG11	1:C:946:LEU:HD13	2.00	0.43
1:E:761:ASN:H	1:E:792:GLY:HA3	1.83	0.43
1:G:889:ARG:HD2	1:G:889:ARG:HA	1.88	0.43
2:B:447:ILE:HD13	2:B:447:ILE:HA	1.75	0.43
1:C:718:THR:HB	1:C:740[B]:ARG:NH2	2.32	0.43
2:D:436:LEU:HD22	2:D:438:HIS:HB3	2.00	0.43
2:D:484:CYS:SG	2:D:490:CYS:HB2	2.58	0.43
1:E:597:ARG:HD2	1:E:733:MET:SD	2.57	0.43
1:E:100:ASN:HB2	2:F:159:ASN:ND2	2.33	0.43
2:F:34:ASP:HB3	2:F:38:ILE:HG21	2.00	0.43
5:C:3071:NAG:C3	5:C:3071:NAG:O7	2.67	0.43
1:C:519:ASP:OD1	1:C:538:HIS:ND1	2.35	0.43
2:F:6:PHE:O	2:F:8:VAL:HG23	2.18	0.43
1:C:692:HIS:HD2	1:G:694:GLU:HA	1.84	0.43
1:A:949:SER:HB3	1:A:1054:THR:OG1	2.19	0.43
2:D:605:SER:O	2:D:609:CYS:HB2	2.18	0.43
1:E:483:ARG:NH2	1:E:941:LEU:O	2.51	0.43
1:A:694:GLU:HA	1:E:692:HIS:CD2	2.53	0.43
1:A:562:LEU:HD23	1:A:562:LEU:HA	1.72	0.43
2:B:300:VAL:HG11	2:B:308:TYR:CE2	2.54	0.43
2:B:329:ASN:OD1	2:B:329:ASN:N	2.51	0.43
2:B:533:GLY:HA3	2:B:551:CYS:SG	2.59	0.43
1:E:1055:PHE:N	1:E:1055:PHE:CD1	2.87	0.43
1:E:956:VAL:HG12	1:E:957:GLU:HG3	1.99	0.43
2:F:505:LYS:HE3	2:F:505:LYS:HB2	1.85	0.43
1:G:1053:ILE:HB	1:G:1070:MET:HB2	2.01	0.43
1:G:376:GLN:HG3	1:G:377:GLU:N	2.34	0.43
1:G:879:ALA:O	1:G:894:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:896:GLN:HG2	1:G:898:GLU:HB3	2.01	0.43
2:H:92:ALA:HA	2:H:391:VAL:O	2.19	0.43
1:A:220:LEU:HA	1:A:220:LEU:HD23	1.81	0.43
1:A:991:PHE:HB2	1:A:1005:ILE:HG21	2.00	0.43
1:C:998:ASN:C	1:C:1000:VAL:H	2.22	0.43
1:C:670:ARG:NH1	1:C:709:THR:O	2.48	0.43
1:C:657:THR:HB	1:C:718:THR:HG22	2.01	0.43
2:D:458:ASN:OD1	2:D:460:GLU:HB3	2.19	0.43
2:D:618:GLY:O	2:D:619:LYS:HB2	2.19	0.43
2:F:145:GLY:HA3	2:F:188:LEU:HD23	2.00	0.43
2:F:476:ARG:HB3	2:F:483:ILE:HA	2.00	0.43
1:G:628:GLN:HG2	1:G:701:PRO:HA	2.00	0.43
1:G:659:ASP:HB2	1:G:716:ASN:OD1	2.19	0.43
1:A:775:LEU:H	1:A:779:ASN:HD22	1.67	0.43
1:E:103:LEU:HD13	1:E:334:GLN:HE21	1.84	0.43
2:F:547:GLU:HG3	2:F:553:CYS:HB2	2.01	0.43
2:F:611:LYS:HD2	2:F:611:LYS:HA	1.77	0.43
1:G:813:VAL:O	1:G:823:ARG:NH1	2.51	0.43
1:A:54:THR:HG22	1:A:56:ALA:N	2.34	0.43
1:C:3:LEU:HB3	1:C:553:ILE:HD11	2.01	0.43
1:C:634:ASN:HD22	1:G:690:LYS:HB3	1.83	0.43
1:E:107:CYS:SG	1:E:336:GLY:HA3	2.59	0.43
1:E:406:PRO:HB3	1:E:438:TYR:CZ	2.54	0.43
1:E:670:ARG:NH2	1:E:709:THR:O	2.51	0.43
2:F:221:VAL:HG11	2:F:237:LEU:HD21	2.01	0.43
1:G:497:HIS:CE1	1:G:528:GLU:H	2.37	0.43
1:G:946:LEU:O	1:G:948:VAL:HG13	2.19	0.43
2:H:125:LYS:O	2:H:196:GLN:NE2	2.46	0.43
2:H:381:VAL:HG21	2:H:387:ILE:HD13	2.00	0.43
1:A:175:SER:OG	1:A:176:ASN:N	2.51	0.43
1:A:410:HIS:O	1:A:436:GLY:N	2.45	0.43
1:A:448:VAL:HA	1:A:518:THR:HB	2.01	0.43
2:B:500:SER:HB3	2:B:505:LYS:HG2	2.00	0.43
1:C:103:LEU:HD12	2:D:156:PRO:HB3	1.99	0.43
1:C:551:GLN:HG3	8:C:4005:HOH:O	2.18	0.43
1:C:601:TRP:CZ2	1:C:643:SER:HA	2.53	0.43
2:D:592:GLU:HG2	2:D:594:PRO:HD3	1.99	0.43
1:E:338:SER:HB2	1:E:388:TYR:O	2.19	0.43
1:E:646:LEU:HD22	1:E:650:ARG:NE	2.33	0.43
1:E:611:ALA:O	1:E:747:PRO:HD2	2.18	0.43
1:G:940:ASN:ND2	1:G:1018:PHE:O	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:ASP:OD1	1:G:4:ASP:C	2.56	0.43
1:G:525:PRO:HA	1:G:532:GLY:HA2	2.01	0.43
1:G:657:THR:HA	1:G:684:VAL:HG22	2.01	0.43
1:A:37:LYS:O	1:A:44:THR:HA	2.19	0.43
1:A:739:GLN:HE21	1:A:741:TYR:HB2	1.84	0.43
1:A:976:SER:O	1:A:978:ARG:N	2.52	0.43
1:E:473:VAL:HG21	1:E:522:ILE:HD13	2.01	0.43
1:E:621:ARG:O	1:E:622:GLU:O	2.37	0.43
1:A:333:ALA:HB2	1:A:353:SER:HB3	2.01	0.42
1:A:4:ASP:HB3	8:A:4001:HOH:O	2.18	0.42
2:B:114:SER:O	2:B:204:ILE:HD11	2.19	0.42
1:C:777:GLY:HA2	1:C:867:PRO:HA	2.01	0.42
1:E:1062:GLN:HE21	1:E:1067:GLU:HA	1.84	0.42
1:E:601:TRP:CZ3	1:E:738:ALA:HB2	2.54	0.42
2:F:472:GLU:HA	2:F:475:CYS:HB2	2.01	0.42
1:A:47:LEU:HD11	1:A:88:ALA:CB	2.49	0.42
1:C:411:THR:OG1	1:C:412:GLY:N	2.52	0.42
1:C:920:ASN:HB2	5:C:3920:NAG:H2	1.99	0.42
2:D:125:LYS:HD3	2:D:200:GLY:HA2	2.00	0.42
2:D:241:THR:O	2:D:300:VAL:HA	2.18	0.42
1:E:411:THR:OG1	1:E:412:GLY:N	2.52	0.42
1:E:525:PRO:HA	1:E:532:GLY:HA2	2.01	0.42
1:E:554:ALA:HB3	1:E:557:GLN:HG3	2.01	0.42
2:H:483:ILE:C	2:H:485:SER:H	2.20	0.42
1:A:37:LYS:HD3	1:A:46:GLY:HA3	2.00	0.42
1:A:741:TYR:CD2	2:B:502:VAL:HG12	2.54	0.42
1:A:838:GLY:N	8:A:4005:HOH:O	2.51	0.42
1:A:848:HIS:CD2	2:B:485:SER:HB3	2.55	0.42
1:A:909:VAL:HB	1:A:1053:ILE:HD11	2.00	0.42
2:B:571:ARG:NH1	2:B:656:GLN:NE2	2.68	0.42
1:C:642:ARG:O	1:C:643:SER:HB3	2.20	0.42
1:C:652:LEU:HD23	1:C:652:LEU:HA	1.88	0.42
6:E:3072:BMA:H61	7:E:3074:MAN:H2	1.57	0.42
1:E:755:ASP:N	1:E:755:ASP:OD1	2.51	0.42
1:E:356:TRP:CH2	2:F:209:ASP:HA	2.54	0.42
5:A:3070:NAG:HO3	5:A:3070:NAG:C7	2.23	0.42
1:A:65:PRO:HA	1:A:66:PRO:HD3	1.92	0.42
1:A:1057:THR:HB	1:C:761:ASN:ND2	2.35	0.42
2:D:547:GLU:HG3	2:D:553:CYS:HB2	2.00	0.42
5:E:3717:NAG:H3	6:E:3718:BMA:O2	2.19	0.42
1:E:623:GLN:HB2	1:E:626:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:670:ARG:NH1	1:G:709:THR:O	2.48	0.42
1:A:1071:ARG:HH21	1:C:755:ASP:CB	2.30	0.42
1:A:525:PRO:HA	1:A:532:GLY:HA2	2.00	0.42
1:C:980:SER:O	1:C:1011:PHE:HA	2.18	0.42
1:G:908:VAL:HG12	1:G:1069:PHE:HB3	2.01	0.42
1:G:847:ASN:O	1:G:849:LEU:N	2.52	0.42
2:H:61:SER:HB3	2:H:91:ALA:HB2	2.02	0.42
1:C:605:SER:O	1:C:635:ILE:HA	2.20	0.42
1:C:35:PRO:O	1:C:72:SER:HA	2.20	0.42
1:C:918:TYR:CZ	1:C:1079:GLU:HB3	2.54	0.42
1:C:918:TYR:HA	1:C:1077:VAL:O	2.19	0.42
1:E:670:ARG:NH1	1:E:709:THR:O	2.51	0.42
1:G:618:PHE:CE1	1:G:707:SER:HB3	2.55	0.42
1:G:803:SER:O	1:G:877:LEU:HA	2.19	0.42
2:H:575:ARG:O	2:H:576:CYS:HB2	2.19	0.42
1:A:501:ARG:O	1:A:524:ALA:HA	2.20	0.42
1:A:940:ASN:HB2	1:A:1018:PHE:CE2	2.55	0.42
1:A:986:PRO:HG3	8:A:4004:HOH:O	2.19	0.42
1:C:638:TYR:HB3	1:C:691:ALA:CB	2.47	0.42
2:D:430:GLN:H	2:D:430:GLN:CD	2.23	0.42
1:E:593:LEU:HD23	1:E:593:LEU:HA	1.71	0.42
1:E:848:HIS:ND1	2:F:485:SER:HB3	2.34	0.42
2:F:518:ASN:O	2:F:538:GLY:HA2	2.20	0.42
1:G:102:TYR:HB2	1:G:331:GLU:O	2.20	0.42
1:G:91:PRO:HG3	1:G:337:PHE:HA	2.02	0.42
1:C:697:ASN:HD21	1:G:653:GLN:HG3	1.85	0.42
2:H:78:PRO:HD2	2:H:95:VAL:HA	2.00	0.42
1:A:649:SER:O	1:A:650:ARG:HB2	2.19	0.42
2:B:173:GLU:HB3	2:B:174:LYS:O	2.20	0.42
2:B:232:ASN:H	2:B:235:ARG:HH21	1.67	0.42
2:B:468:SER:O	2:B:472:GLU:HG3	2.19	0.42
2:B:518:ASN:O	2:B:538:GLY:HA2	2.19	0.42
1:C:849:LEU:HA	1:C:849:LEU:HD23	1.77	0.42
2:D:591:GLN:HG3	2:D:592:GLU:N	2.34	0.42
1:E:848:HIS:CG	2:F:485:SER:HB3	2.54	0.42
2:F:281:SER:OG	2:F:284:GLN:HB2	2.19	0.42
2:F:317:LYS:HD2	2:F:317:LYS:HA	1.90	0.42
2:F:643:ARG:HA	2:F:649:TRP:HA	2.02	0.42
1:G:717:PHE:N	1:G:717:PHE:CD1	2.88	0.42
1:G:1:PHE:CZ	1:G:735:ALA:HA	2.54	0.42
1:G:902:LYS:NZ	1:G:1058:SER:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:495:CYS:HB2	2:H:510:GLN:O	2.20	0.42
1:A:606:MET:HB3	1:A:744:ALA:HB2	2.00	0.42
1:A:811:ARG:HB2	1:A:864:ASP:OD2	2.20	0.42
1:C:12:ARG:HD2	1:C:590:GLN:NE2	2.34	0.42
2:D:183:ARG:HG3	2:D:184:HIS:O	2.20	0.42
1:E:376:GLN:HA	5:E:3373:NAG:C7	2.49	0.42
1:A:957:GLU:OE2	1:A:960:GLN:HA	2.20	0.42
2:B:382:GLN:OE1	2:B:385:VAL:HG21	2.20	0.42
2:B:522:TYR:CD1	2:B:552:GLN:HA	2.55	0.42
5:C:3717:NAG:O7	5:C:3717:NAG:C3	2.68	0.42
1:C:392:LEU:HD11	1:C:399:GLN:HB2	2.01	0.42
1:C:600:LEU:HD23	1:C:601:TRP:CH2	2.55	0.42
1:E:965:MET:N	1:E:1031:ASN:O	2.52	0.42
1:E:625:VAL:HG12	1:E:628:GLN:HG3	2.02	0.42
2:F:589:LEU:HD23	2:F:589:LEU:HA	1.85	0.42
2:H:644:ASP:HB3	2:H:650:VAL:HG23	2.00	0.42
1:A:1069:PHE:N	1:A:1069:PHE:CD1	2.88	0.41
1:A:173:GLN:HB3	1:A:181:HIS:HE1	1.84	0.41
1:A:301:ASP:O	1:A:304:LYS:HG2	2.19	0.41
2:B:105:ILE:HG13	2:B:234:THR:HB	2.02	0.41
2:B:136:ASN:HA	2:B:139:THR:O	2.20	0.41
1:C:407:ARG:NH1	2:D:246:HIS:HA	2.35	0.41
2:D:150:VAL:HB	2:D:180:PHE:O	2.20	0.41
2:D:434:ARG:HG2	2:D:434:ARG:HH11	1.84	0.41
2:D:468:SER:HB3	2:D:471:LEU:HD12	2.02	0.41
2:D:97:PHE:CE2	2:D:345:VAL:HG21	2.54	0.41
2:F:316:PRO:HB3	2:F:346:PHE:CE1	2.55	0.41
2:F:399:ILE:HG13	2:F:399:ILE:H	1.69	0.41
1:C:694:GLU:HA	1:G:692:HIS:CD2	2.55	0.41
1:G:730:LEU:H	1:G:730:LEU:HG	1.59	0.41
1:A:920:ASN:OD1	1:A:920:ASN:C	2.59	0.41
2:B:7:LYS:O	2:B:13:GLU:HB3	2.20	0.41
1:C:456:LEU:HD13	1:C:475:VAL:HG13	2.02	0.41
2:D:230:TRP:CZ3	2:D:235:ARG:HB3	2.55	0.41
2:D:6:PHE:O	2:D:8:VAL:HG23	2.20	0.41
1:E:1052:GLU:CD	1:E:1071[B]:ARG:HH11	2.23	0.41
1:E:538:HIS:CD2	1:E:550:SER:OG	2.73	0.41
1:G:1066:GLN:H	1:G:1066:GLN:CD	2.23	0.41
1:G:347:VAL:HG21	1:G:401:LEU:HD11	2.02	0.41
1:G:713:LEU:O	1:G:743:THR:HA	2.20	0.41
1:G:726:ALA:C	1:G:728:ARG:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:729:ASN:HD22	1:G:729:ASN:H	1.67	0.41
2:H:447:ILE:HD13	2:H:447:ILE:HA	1.93	0.41
1:A:442:SER:OG	1:A:504:ALA:O	2.32	0.41
2:B:598:SER:HA	2:B:599:PRO:HD3	1.76	0.41
1:E:16:ALA:HB1	1:E:36:GLN:HB2	2.02	0.41
1:E:564:TYR:CD2	1:E:588:ARG:HD2	2.55	0.41
2:F:361:ASP:HA	2:F:371:ARG:HA	2.02	0.41
6:G:3072:BMA:O4	7:G:3074:MAN:H2	2.20	0.41
1:A:908:VAL:HA	1:A:1069:PHE:O	2.19	0.41
2:B:484:CYS:SG	2:B:490:CYS:HB2	2.60	0.41
2:B:635:VAL:HB	2:B:655:GLU:OE1	2.20	0.41
1:C:686:VAL:HG11	1:G:697:ASN:HD21	1.86	0.41
2:D:613:GLU:O	2:D:614:LYS:HD2	2.20	0.41
1:E:971:HIS:HE1	1:E:1024:LEU:HB3	1.85	0.41
1:E:564:TYR:HB3	1:E:567:GLN:OE1	2.20	0.41
1:G:660:LEU:HB3	1:G:713:LEU:HD11	2.02	0.41
1:G:836:SER:O	1:G:837:GLN:HB2	2.21	0.41
2:H:363:PHE:HB2	2:H:388:THR:HB	2.02	0.41
1:A:765:SER:HA	1:A:895:PHE:CD2	2.56	0.41
1:A:385:TYR:CZ	2:B:253:LEU:HD11	2.56	0.41
1:C:897:LEU:HD12	1:C:897:LEU:HA	1.85	0.41
1:C:96:GLU:HG2	1:C:98:GLY:H	1.85	0.41
1:E:334:GLN:NE2	2:F:253:LEU:O	2.53	0.41
1:G:115:LEU:H	1:G:115:LEU:CD2	2.34	0.41
5:G:3881:NAG:H83	5:G:3881:NAG:C3	2.50	0.41
2:H:604:ILE:HA	2:H:604:ILE:HD13	1.82	0.41
2:H:6:PHE:O	2:H:8:VAL:HG23	2.20	0.41
1:A:1051:ALA:O	1:A:1071:ARG:HA	2.21	0.41
1:A:181:HIS:CD2	1:A:200:VAL:HG13	2.56	0.41
1:A:384:SER:O	1:A:385:TYR:HB2	2.20	0.41
2:B:146:PHE:HD2	2:B:185:VAL:HG21	1.85	0.41
1:C:887:THR:OG1	1:C:888:PRO:HD2	2.21	0.41
2:D:611:LYS:HG2	2:D:667:VAL:HB	2.03	0.41
2:F:104:PRO:HB2	2:F:233:VAL:HG11	2.02	0.41
1:G:512:VAL:HG22	1:G:519:ASP:OD2	2.20	0.41
1:C:599:VAL:HG12	1:C:601:TRP:CD1	2.55	0.41
1:C:618:PHE:HB2	1:C:704:VAL:HG22	2.03	0.41
1:C:713:LEU:O	1:C:743:THR:HA	2.20	0.41
1:C:797:GLY:HA3	1:C:884:GLU:HG3	2.03	0.41
2:D:460:GLU:HG2	2:D:461:CYS:N	2.36	0.41
1:E:716:ASN:HB3	1:E:741:TYR:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:905:VAL:HG11	1:E:946:LEU:HD22	2.02	0.41
1:G:933:MET:HA	1:G:1028:LEU:O	2.21	0.41
1:A:952:PHE:HB2	1:A:1011:PHE:HB2	2.03	0.41
1:A:70:ASN:N	1:A:70:ASN:OD1	2.53	0.41
2:B:604:ILE:HG12	2:B:642:GLU:HG3	2.03	0.41
1:C:347:VAL:HA	1:C:361:PHE:O	2.21	0.41
1:C:374:MET:HB3	1:C:378:ASN:ND2	2.35	0.41
1:C:875:LEU:O	1:C:898:GLU:HA	2.21	0.41
2:D:469:GLN:C	2:D:471:LEU:N	2.74	0.41
1:E:526:GLY:HA2	1:E:530:ASN:HA	2.03	0.41
1:G:476:CYS:HA	1:G:487:CYS:HA	2.03	0.41
1:G:535:TYR:HB3	1:G:537:PHE:HE1	1.85	0.41
2:H:189:THR:OG1	2:H:190:ASN:N	2.46	0.41
5:A:3880:NAG:C7	5:A:3880:NAG:HO3	2.26	0.41
1:A:639:ILE:HG23	1:A:639:ILE:O	2.21	0.41
1:C:874:ARG:HA	1:C:899:LEU:O	2.21	0.41
1:C:93:VAL:HB	1:C:104:THR:O	2.21	0.41
2:D:571:ARG:O	2:D:582:HIS:ND1	2.54	0.41
2:F:184:HIS:CE1	2:F:228:ILE:HG12	2.56	0.41
1:G:1048:VAL:HG11	1:G:1073:GLN:HE21	1.86	0.41
1:G:649:SER:O	1:G:651:ASP:N	2.50	0.41
1:G:47:LEU:HG	1:G:73:LEU:HD13	2.03	0.41
1:A:970:SER:HB3	1:A:1027:THR:OG1	2.19	0.41
2:B:97:PHE:O	2:B:386:PRO:HA	2.21	0.41
2:B:505:LYS:HD2	2:B:517:ILE:HD12	2.03	0.41
1:E:813:VAL:O	1:E:823:ARG:NH1	2.53	0.41
1:E:954:VAL:HG13	1:E:964:TRP:CE3	2.56	0.41
1:G:918:TYR:CA	1:G:1077:VAL:HB	2.51	0.41
1:G:625:VAL:HG12	1:G:625:VAL:O	2.20	0.41
1:A:307:GLN:O	1:A:311:LYS:HG3	2.21	0.41
1:A:12:ARG:HA	1:A:590:GLN:HB3	2.03	0.41
1:C:1020:VAL:HG12	1:C:1021:GLN:HG2	2.02	0.41
2:D:624:ALA:CB	5:D:3620:NAG:H82	2.51	0.41
5:E:3880:NAG:H83	5:E:3880:NAG:H3	2.01	0.41
1:E:969:VAL:HG22	1:E:1028:LEU:HD23	2.03	0.41
2:F:35:PRO:O	2:F:38:ILE:HG12	2.19	0.41
1:G:1044:LYS:HE3	1:G:1044:LYS:HB3	1.90	0.41
5:G:3042:NAG:H2	5:G:3070:NAG:H83	2.01	0.41
1:G:448:VAL:HA	1:G:518:THR:HB	2.02	0.41
1:A:413:LYS:HG3	1:A:430:VAL:O	2.22	0.40
1:A:9:THR:HG21	1:A:52:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:HIS:HB3	2:B:281:SER:HB2	2.02	0.40
2:B:242:ASP:HA	2:B:301:THR:OG1	2.21	0.40
1:C:931:VAL:HA	1:C:1031:ASN:HA	2.02	0.40
1:C:38:ILE:HG12	5:C:3070:NAG:H83	2.02	0.40
1:C:67:GLU:N	1:C:67:GLU:OE1	2.45	0.40
1:C:918:TYR:CE2	1:C:920:ASN:HB3	2.56	0.40
2:D:430:GLN:N	2:D:430:GLN:OE1	2.49	0.40
1:E:998:ASN:C	1:E:1000:VAL:H	2.24	0.40
1:E:481:GLY:HA2	1:E:1021:GLN:HB3	2.02	0.40
1:E:564:TYR:HD2	1:E:588:ARG:HB2	1.86	0.40
1:E:575:LEU:N	1:E:582:ASP:OD2	2.54	0.40
1:E:963:VAL:HG13	1:E:1036:TRP:NE1	2.35	0.40
1:G:917:LYS:HA	1:G:1076:THR:HA	2.03	0.40
1:G:810:TYR:HB2	1:G:842:THR:HG21	2.02	0.40
5:H:3232:NAG:H83	5:H:3232:NAG:H3	2.02	0.40
2:H:358:VAL:HG22	2:H:393:VAL:HG22	2.03	0.40
1:C:800:ILE:O	1:C:844:CYS:N	2.53	0.40
1:C:961:GLU:OE1	1:C:1039:GLN:HG3	2.21	0.40
2:D:570:GLY:HA3	2:D:659:GLY:CA	2.51	0.40
1:E:635:ILE:O	1:E:693:CYS:HA	2.21	0.40
2:H:238:VAL:HG22	2:H:297:ILE:HB	2.03	0.40
1:A:1030:GLY:HA2	1:G:113:THR:HG22	2.03	0.40
1:A:173:GLN:NE2	1:A:203:LEU:H	2.18	0.40
1:A:739:GLN:NE2	1:A:741:TYR:HB2	2.36	0.40
2:D:571:ARG:HG3	2:D:660:MET:HE3	2.03	0.40
2:F:164:LYS:HA	2:F:164:LYS:HD2	1.88	0.40
2:F:266:LEU:HA	2:F:270:LEU:O	2.21	0.40
2:F:637:GLY:HA3	2:F:654:LEU:O	2.22	0.40
1:G:470:GLY:HA3	1:G:498:PRO:O	2.21	0.40
1:G:774:LEU:HD23	1:G:901:VAL:HG22	2.04	0.40
2:B:315:ILE:O	2:B:315:ILE:HG23	2.21	0.40
1:A:917:LYS:HZ1	2:B:642:GLU:HB3	1.83	0.40
2:D:221:VAL:HG11	2:D:237:LEU:HD21	2.02	0.40
1:E:582:ASP:OD1	1:E:595:ARG:HG2	2.22	0.40
1:G:959:ASN:O	1:G:960:GLN:HB2	2.22	0.40
1:A:136:LEU:HB2	1:A:235:LEU:HD11	2.02	0.40
1:A:338:SER:HB2	1:A:388:TYR:O	2.21	0.40
1:A:603:GLY:HA3	1:A:638:TYR:CZ	2.56	0.40
2:B:223:ALA:O	2:B:264:CYS:HB2	2.20	0.40
1:C:823:ARG:HD2	1:C:860:LEU:O	2.21	0.40
2:D:31:GLY:H	2:D:34:ASP:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:66:GLN:O	2:D:80:LYS:HB3	2.21	0.40
1:E:384:SER:HB2	1:E:405:ALA:HB1	2.03	0.40
1:E:714:ARG:HG2	1:E:715:LEU:N	2.37	0.40
2:F:598:SER:O	2:F:600:CYS:N	2.53	0.40
1:G:918:TYR:N	1:G:1077:VAL:HB	2.37	0.40
1:G:605:SER:HB3	1:G:636:CYS:HB2	2.03	0.40
1:G:804:HIS:CD2	1:G:863:PHE:CE2	3.09	0.40
2:H:285:LEU:HA	2:H:285:LEU:HD23	1.82	0.40

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

All (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
2	B	621	CYS
1	C	624	VAL
1	C	643	SER
1	C	644	LYS
1	C	772	LYS
1	C	921	PHE
2	D	104	PRO
2	D	233	VAL
2	D	588	PRO
1	E	622	GLU
1	E	643	SER
1	E	652	LEU
1	E	920	ASN
2	F	272	LYS
1	G	396	LYS
1	G	482	TRP
1	G	640	ASP
1	G	837	GLN
1	G	848	HIS
1	G	894	THR
1	G	921	PHE
2	H	452	THR
2	H	619	LYS
2	H	620	ASN
1	A	70	ASN
1	A	175	SER
1	A	324	SER
1	A	397	GLY
1	A	921	PHE
1	A	922	SER
1	C	42	ASN
1	C	449	ASP
1	C	621	ARG
1	C	646	LEU
1	C	728	ARG
1	C	818	LYS
2	D	73	GLN

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Mol	Chain	Res	Type
2	D	229	GLY
2	D	231	ARG
2	D	435	SER
1	E	82	SER
1	E	98	GLY
1	E	758	CYS
1	E	818	LYS
1	E	853	GLY
1	E	1018	PHE
2	F	435	SER
2	F	601	GLY
1	G	625	VAL
1	G	648	GLY
1	G	652	LEU
1	G	769	PRO
2	H	487	LEU
1	A	229	ARG
1	A	644	LYS
2	B	558	GLU
1	C	4	ASP
1	C	16	ALA
1	C	82	SER
1	C	560	SER
1	C	640	ASP
1	C	731	ARG
1	C	798	THR
1	C	890	THR
1	E	623	GLN
1	E	772	LYS
1	E	894	THR
1	G	16	ALA
1	G	641	LYS
1	G	772	LYS
1	G	853	GLY
1	G	920	ASN
2	H	466	ARG
2	H	600	CYS
1	A	206	PHE
1	A	323	THR
1	A	385	TYR
1	A	918	TYR
1	A	972	PRO

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Mol	Chain	Res	Type
1	A	1021	GLN
2	B	232	ASN
2	B	588	PRO
2	D	470	GLU
1	E	626	SER
1	E	671	ALA
2	F	506	LEU
2	F	588	PRO
1	G	35	PRO
1	G	887	THR
1	G	922	SER
2	H	576	CYS
1	A	723	PRO
1	A	977	LEU
1	C	483	ARG
1	E	396	LYS
1	E	1021	GLN
1	G	82	SER
2	H	186	LEU
2	H	621	CYS
1	A	504	ALA
1	C	652	LEU
1	C	770	GLY
2	D	583	SER
1	E	731	ARG
1	E	999	PRO
2	H	233	VAL
1	A	625	VAL
1	E	397	GLY
2	F	594	PRO
1	A	340	VAL
1	C	479	PRO
2	F	595	GLY
2	F	625	CYS
1	G	963	VAL

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

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	618	PHE
1	A	625	VAL
1	A	630	LEU
1	A	771	LEU
1	A	808	LEU
1	A	834	VAL
1	A	859	PHE
1	A	899	LEU
1	A	959	ASN
1	A	964	TRP
1	A	1021	GLN
2	B	73	GLN
2	B	232	ASN
2	B	247	PHE
2	B	266	LEU
2	B	268	ASP
2	B	502	VAL
2	B	598	SER
1	C	70	ASN
1	C	101	MET
1	C	394	LEU
1	C	480	ARG
1	C	595	ARG
1	C	601	TRP

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Mol	Chain	Res	Type
1	C	625	VAL
1	C	630	LEU
1	C	638	TYR
1	C	690	LYS
1	C	716	ASN
1	C	921	PHE
2	D	11	CYS
2	D	231	ARG
2	D	435	SER
2	D	437	CYS
2	D	438	HIS
2	D	445	CYS
2	D	462	GLN
2	D	621	CYS
1	E	70	ASN
1	E	73	LEU
1	E	388	TYR
1	E	395	TRP
1	E	616	SER
1	E	638	TYR
1	E	644	LYS
1	E	650	ARG
1	E	717	PHE
1	E	730	LEU
1	E	750	LYS
1	E	758	CYS
1	E	774	LEU
1	E	899	LEU
1	E	946	LEU
1	E	964	TRP
1	E	1055	PHE
2	F	110	LEU
2	F	155	LEU
2	F	247	PHE
2	F	425	CYS
1	G	4	ASP
1	G	73	LEU
1	G	101	MET
1	G	115	LEU
1	G	638	TYR
1	G	717	PHE
1	G	729	ASN

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Mol	Chain	Res	Type
1	G	804	HIS
1	G	808	LEU
1	G	849	LEU
1	G	919	LEU
1	G	920	ASN
1	G	923	GLU
1	G	924	SER
1	G	939	ASN
1	G	1055	PHE
2	H	224	CYS
2	H	492	CYS
2	H	506	LEU
2	H	571	ARG
2	H	621	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	94	HIS
1	A	114	GLN
1	A	173	GLN
1	A	181	HIS
1	A	697	ASN
1	A	751	ASN
1	A	779	ASN
1	A	848	HIS
1	A	951	ASN
2	B	45	GLN
2	B	167	ASN
2	B	287	HIS
2	B	292	ASN
2	B	400	GLN
2	B	657	GLN
1	C	43	GLN
1	C	590	GLN
1	C	930	HIS
2	D	89	GLN
2	D	438	HIS
1	E	410	HIS
1	E	653	GLN
1	E	697	ASN

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Mol	Chain	Res	Type
1	E	779	ASN
1	E	971	HIS
2	F	45	GLN
1	G	378	ASN
1	G	495	GLN
1	G	692	HIS
1	G	697	ASN
1	G	779	ASN
1	G	848	HIS
1	G	939	ASN
1	G	960	GLN
1	G	994	HIS
1	G	1066	GLN
1	G	1073	GLN
2	H	159	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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
6	E	3072	BMA	O5-C1	-4.16	1.36	1.43
5	H	3190	NAG	O5-C1	-4.14	1.37	1.43
5	G	3880	NAG	O5-C1	-3.99	1.37	1.43
5	A	3374	NAG	O5-C1	-3.90	1.37	1.43
6	A	3718	BMA	O5-C1	-3.81	1.37	1.43
7	E	3074	MAN	O5-C1	-3.77	1.37	1.43
5	E	3880	NAG	O5-C1	-3.75	1.37	1.43
5	C	3070	NAG	O5-C1	-3.58	1.37	1.43
5	E	3716	NAG	O5-C1	-3.36	1.38	1.43
5	B	3232	NAG	O5-C1	-3.36	1.38	1.43
6	C	3375	BMA	O5-C1	-3.27	1.38	1.43
5	G	3920	NAG	O5-C1	-3.13	1.38	1.43
5	C	3071	NAG	O5-C1	-2.99	1.38	1.43
6	G	3882	BMA	O5-C1	-2.94	1.38	1.43
5	E	3071	NAG	C1-C2	-2.84	1.48	1.52
7	G	3719	MAN	O5-C1	-2.78	1.39	1.43
6	E	3072	BMA	O5-C5	-2.73	1.37	1.43
6	E	3072	BMA	C6-C5	-2.73	1.42	1.51
5	C	3373	NAG	O5-C1	-2.71	1.39	1.43
6	G	3375	BMA	O4-C4	-2.66	1.36	1.43
5	G	3678	NAG	O5-C1	-2.64	1.39	1.43
5	E	3717	NAG	O5-C1	-2.58	1.39	1.43
7	G	3379	MAN	O5-C1	-2.54	1.39	1.43
5	A	3678	NAG	O5-C1	-2.53	1.39	1.43
7	E	3719	MAN	O5-C1	-2.50	1.39	1.43
7	A	3377	MAN	O5-C1	-2.50	1.39	1.43
5	E	3881	NAG	O5-C1	-2.46	1.39	1.43
5	G	3717	NAG	O5-C1	-2.41	1.39	1.43
5	E	3071	NAG	O5-C1	-2.37	1.39	1.43
7	C	3376	MAN	O5-C1	-2.34	1.39	1.43
6	G	3718	BMA	C2-C3	-2.24	1.49	1.52
5	A	3880	NAG	O5-C1	-2.21	1.40	1.43
5	G	3881	NAG	O5-C1	-2.18	1.40	1.43
6	E	3375	BMA	O5-C1	-2.12	1.40	1.43
5	E	3070	NAG	O5-C1	-2.06	1.40	1.43
5	H	3094	NAG	O5-C1	-2.02	1.40	1.43
7	G	3376	MAN	O2-C2	2.03	1.47	1.43
7	C	3719	MAN	C2-C3	2.04	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3380	MAN	C1-C2	2.04	1.57	1.52
7	A	3376	MAN	C2-C3	2.05	1.55	1.52
7	C	3377	MAN	C1-C2	2.07	1.57	1.52
5	C	3678	NAG	C1-C2	2.15	1.55	1.52
6	E	3072	BMA	O3-C3	2.16	1.48	1.43
5	C	3920	NAG	C1-C2	2.18	1.55	1.52
7	C	3378	MAN	O5-C5	2.18	1.48	1.43
7	C	3377	MAN	C4-C3	2.19	1.58	1.52
7	G	3884	MAN	C2-C3	2.20	1.55	1.52
7	G	3073	MAN	C1-C2	2.23	1.57	1.52
7	G	3883	MAN	O5-C5	2.24	1.48	1.43
5	E	3920	NAG	O5-C1	2.25	1.47	1.43
5	C	3042	NAG	O5-C1	2.26	1.47	1.43
6	G	3375	BMA	C1-C2	2.28	1.57	1.52
7	C	3720	MAN	C1-C2	2.29	1.57	1.52
6	E	3718	BMA	C1-C2	2.33	1.57	1.52
6	E	3072	BMA	C4-C5	2.34	1.58	1.53
5	A	3042	NAG	O5-C1	2.35	1.47	1.43
6	A	3718	BMA	C4-C3	2.37	1.58	1.52
7	C	3884	MAN	C2-C3	2.38	1.55	1.52
7	A	3376	MAN	C4-C3	2.39	1.58	1.52
7	C	3378	MAN	C1-C2	2.40	1.58	1.52
5	A	3920	NAG	C1-C2	2.44	1.55	1.52
7	E	3074	MAN	O5-C5	2.45	1.48	1.43
7	A	3382	MAN	C1-C2	2.48	1.58	1.52
6	E	3882	BMA	O6-C6	2.48	1.53	1.42
6	A	3072	BMA	C4-C3	2.52	1.59	1.52
6	G	3375	BMA	C4-C3	2.53	1.59	1.52
6	E	3882	BMA	C1-C2	2.54	1.58	1.52
5	C	3716	NAG	C1-C2	2.58	1.56	1.52
7	C	3380	MAN	O5-C5	2.62	1.49	1.43
6	A	3072	BMA	C4-C5	2.62	1.58	1.53
6	E	3072	BMA	C2-C3	2.63	1.56	1.52
5	H	3232	NAG	O5-C1	2.65	1.48	1.43
6	C	3072	BMA	C4-C3	2.68	1.59	1.52
7	C	3884	MAN	C1-C2	2.72	1.58	1.52
7	C	3719	MAN	O3-C3	2.73	1.49	1.43
6	C	3882	BMA	C4-C3	2.73	1.59	1.52
7	C	3884	MAN	O5-C1	2.76	1.48	1.43
6	A	3375	BMA	C2-C3	2.76	1.56	1.52
6	E	3882	BMA	C6-C5	2.81	1.61	1.51
7	G	3884	MAN	C1-C2	2.83	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	3232	NAG	C1-C2	2.87	1.56	1.52
5	G	3042	NAG	C1-C2	2.88	1.56	1.52
7	A	3379	MAN	C1-C2	2.88	1.59	1.52
7	C	3884	MAN	O5-C5	2.99	1.50	1.43
6	C	3375	BMA	C2-C3	3.10	1.56	1.52
5	C	3042	NAG	C1-C2	3.13	1.56	1.52
7	G	3376	MAN	C1-C2	3.16	1.59	1.52
7	G	3376	MAN	C2-C3	3.33	1.57	1.52
6	C	3375	BMA	O3-C3	3.38	1.50	1.43
5	B	3094	NAG	C1-C2	3.49	1.57	1.52
7	E	3074	MAN	O2-C2	3.54	1.51	1.43
7	E	3884	MAN	O5-C1	3.68	1.49	1.43
7	C	3377	MAN	C2-C3	3.84	1.57	1.52
7	C	3377	MAN	O2-C2	3.91	1.52	1.43
6	C	3072	BMA	C1-C2	3.99	1.62	1.52
7	A	3380	MAN	C2-C3	4.04	1.58	1.52
6	C	3375	BMA	C1-C2	4.11	1.62	1.52
7	E	3074	MAN	C1-C2	4.42	1.63	1.52
7	E	3074	MAN	C2-C3	4.98	1.59	1.52
7	E	3884	MAN	O5-C5	5.79	1.56	1.43

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
5	B	3094	NAG	C2-N2-C7	-4.29	117.53	123.11
6	A	3375	BMA	O5-C5-C6	-4.04	98.70	107.34
6	G	3718	BMA	O2-C2-C3	-3.78	102.57	110.19
6	C	3375	BMA	C2-C3-C4	-3.62	104.74	111.05
6	C	3072	BMA	O2-C2-C3	-3.59	102.95	110.19
7	E	3074	MAN	O2-C2-C3	-3.45	103.23	110.19
7	A	3376	MAN	O2-C2-C3	-3.45	103.24	110.19
6	E	3882	BMA	O2-C2-C3	-3.01	104.11	110.19
6	E	3718	BMA	O2-C2-C3	-3.00	104.15	110.19
7	G	3884	MAN	O2-C2-C3	-2.96	104.21	110.19
6	G	3375	BMA	C2-C3-C4	-2.96	105.88	111.05
6	G	3375	BMA	O4-C4-C5	-2.94	101.47	109.23
7	G	3380	MAN	O2-C2-C3	-2.91	104.33	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	3073	MAN	O2-C2-C3	-2.90	104.34	110.19
7	C	3380	MAN	O2-C2-C3	-2.88	104.39	110.19
5	B	3094	NAG	O4-C4-C3	-2.81	104.02	110.36
7	C	3073	MAN	O2-C2-C3	-2.78	104.59	110.19
5	A	3071	NAG	C4-C3-C2	-2.74	107.09	111.34
6	C	3375	BMA	C1-C2-C3	-2.72	106.26	109.55
6	G	3375	BMA	C1-C2-C3	-2.66	106.33	109.55
5	C	3374	NAG	C4-C3-C2	-2.66	107.21	111.34
7	A	3377	MAN	O2-C2-C3	-2.62	104.90	110.19
7	A	3379	MAN	O2-C2-C3	-2.62	104.90	110.19
7	A	3380	MAN	O5-C5-C4	-2.57	105.87	110.13
5	A	3880	NAG	C1-O5-C5	-2.57	108.36	112.14
5	E	3880	NAG	O4-C4-C3	-2.57	104.57	110.36
7	E	3380	MAN	O2-C2-C3	-2.56	105.03	110.19
7	G	3073	MAN	O2-C2-C3	-2.56	105.03	110.19
6	C	3072	BMA	O6-C6-C5	-2.50	102.94	111.30
6	E	3072	BMA	O5-C1-C2	-2.47	106.94	110.89
6	E	3072	BMA	C1-O5-C5	-2.46	108.53	112.14
5	C	3071	NAG	O3-C3-C2	-2.44	104.15	109.37
7	E	3883	MAN	O2-C2-C3	-2.44	105.27	110.19
7	E	3075	MAN	O2-C2-C3	-2.43	105.29	110.19
7	A	3382	MAN	O2-C2-C3	-2.42	105.31	110.19
6	G	3375	BMA	C1-O5-C5	-2.41	108.59	112.14
6	C	3882	BMA	O2-C2-C3	-2.40	105.36	110.19
6	A	3375	BMA	O6-C6-C5	-2.39	103.33	111.30
5	B	3094	NAG	C1-O5-C5	-2.38	108.64	112.14
6	C	3072	BMA	C1-O5-C5	-2.37	108.65	112.14
7	A	3378	MAN	O2-C2-C3	-2.37	105.40	110.19
6	G	3072	BMA	O2-C2-C3	-2.37	105.41	110.19
5	G	3374	NAG	C4-C3-C2	-2.37	107.66	111.34
6	C	3718	BMA	O2-C2-C3	-2.37	105.42	110.19
6	E	3072	BMA	O5-C5-C6	-2.31	102.40	107.34
7	E	3884	MAN	O2-C2-C3	-2.31	105.54	110.19
7	A	3719	MAN	O2-C2-C3	-2.30	105.54	110.19
5	E	3071	NAG	O3-C3-C2	-2.30	104.45	109.37
7	E	3073	MAN	O2-C2-C3	-2.30	105.55	110.19
7	C	3884	MAN	O2-C2-C3	-2.30	105.56	110.19
5	B	3094	NAG	O5-C5-C4	-2.29	106.35	110.13
7	C	3720	MAN	O2-C2-C3	-2.26	105.62	110.19
7	C	3376	MAN	O2-C2-C3	-2.26	105.62	110.19
6	E	3375	BMA	O2-C2-C3	-2.25	105.66	110.19
7	G	3719	MAN	O2-C2-C3	-2.24	105.66	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	3718	BMA	O2-C2-C3	-2.24	105.68	110.19
7	E	3719	MAN	O2-C2-C3	-2.23	105.68	110.19
6	G	3375	BMA	O2-C2-C3	-2.21	105.73	110.19
5	C	3374	NAG	C3-C4-C5	-2.21	106.29	110.23
7	G	3379	MAN	O2-C2-C3	-2.18	105.80	110.19
5	A	3071	NAG	C3-C4-C5	-2.16	106.38	110.23
6	E	3072	BMA	O3-C3-C4	-2.14	105.54	110.36
5	C	3071	NAG	O4-C4-C3	-2.14	105.54	110.36
7	A	3376	MAN	O5-C5-C4	-2.13	106.61	110.13
6	G	3882	BMA	O2-C2-C3	-2.12	105.92	110.19
7	G	3380	MAN	O6-C6-C5	-2.10	104.30	111.30
6	A	3882	BMA	O2-C2-C3	-2.08	105.99	110.19
7	A	3381	MAN	C1-C2-C3	-2.07	107.04	109.55
6	G	3718	BMA	O4-C4-C3	-2.05	105.73	110.36
5	G	3373	NAG	O3-C3-C2	-2.03	105.04	109.37
7	E	3380	MAN	O5-C1-C2	2.00	114.10	110.89
7	C	3378	MAN	O2-C2-C1	2.01	113.27	109.23
7	G	3377	MAN	O5-C1-C2	2.05	114.17	110.89
7	C	3073	MAN	C1-O5-C5	2.05	115.16	112.14
6	E	3882	BMA	O2-C2-C1	2.07	113.38	109.23
5	C	3071	NAG	O5-C5-C4	2.09	113.60	110.13
7	E	3074	MAN	O3-C3-C2	2.10	113.85	110.01
7	C	3376	MAN	C1-O5-C5	2.10	115.23	112.14
6	G	3375	BMA	O2-C2-C1	2.12	113.47	109.23
7	C	3883	MAN	C1-C2-C3	2.12	112.12	109.55
7	G	3883	MAN	O5-C1-C2	2.12	114.29	110.89
5	A	3374	NAG	O5-C5-C4	2.16	113.72	110.13
5	E	3373	NAG	C2-N2-C7	2.18	125.95	123.11
5	H	3190	NAG	C1-O5-C5	2.19	115.36	112.14
5	E	3071	NAG	O5-C5-C4	2.19	113.77	110.13
6	E	3718	BMA	O2-C2-C1	2.20	113.65	109.23
5	B	3094	NAG	C4-C3-C2	2.23	114.80	111.34
6	C	3072	BMA	O5-C5-C6	2.23	112.12	107.34
7	A	3380	MAN	O3-C3-C2	2.24	114.11	110.01
7	A	3073	MAN	O5-C1-C2	2.26	114.50	110.89
6	E	3375	BMA	C1-C2-C3	2.26	112.29	109.55
7	A	3074	MAN	C1-O5-C5	2.28	115.49	112.14
7	G	3884	MAN	O5-C1-C2	2.32	114.61	110.89
5	H	3620	NAG	C1-O5-C5	2.37	115.63	112.14
5	G	3880	NAG	O5-C5-C4	2.39	114.09	110.13
7	G	3884	MAN	C1-C2-C3	2.39	112.45	109.55
7	E	3380	MAN	C1-C2-C3	2.41	112.47	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	3072	BMA	O3-C3-C2	2.41	114.43	110.01
5	A	3071	NAG	O3-C3-C4	2.43	115.83	110.36
6	E	3882	BMA	O5-C1-C2	2.44	114.80	110.89
7	E	3074	MAN	C1-C2-C3	2.46	112.54	109.55
7	A	3073	MAN	C1-C2-C3	2.46	112.54	109.55
7	C	3884	MAN	O5-C1-C2	2.47	114.84	110.89
5	E	3070	NAG	O4-C4-C3	2.53	116.06	110.36
6	A	3072	BMA	O2-C2-C1	2.57	114.37	109.23
5	A	3071	NAG	C1-O5-C5	2.57	115.92	112.14
7	E	3073	MAN	C1-O5-C5	2.59	115.95	112.14
7	C	3378	MAN	C1-C2-C3	2.60	112.70	109.55
5	E	3881	NAG	C2-N2-C7	2.61	126.50	123.11
6	E	3718	BMA	O5-C1-C2	2.62	115.08	110.89
7	A	3719	MAN	O5-C1-C2	2.62	115.09	110.89
5	C	3678	NAG	C2-N2-C7	2.64	126.54	123.11
6	C	3718	BMA	C1-O5-C5	2.65	116.04	112.14
6	G	3375	BMA	O5-C5-C6	2.66	113.04	107.34
6	E	3375	BMA	C1-O5-C5	2.70	116.11	112.14
7	C	3377	MAN	C1-O5-C5	2.71	116.13	112.14
7	A	3379	MAN	O5-C1-C2	2.75	115.30	110.89
5	A	3071	NAG	O4-C4-C3	2.80	116.68	110.36
7	E	3883	MAN	C1-O5-C5	2.82	116.28	112.14
5	G	3880	NAG	C2-N2-C7	2.82	126.77	123.11
7	G	3073	MAN	C1-C2-C3	2.84	112.99	109.55
5	G	3374	NAG	O3-C3-C4	2.89	116.87	110.36
7	A	3381	MAN	C1-O5-C5	2.95	116.48	112.14
7	E	3884	MAN	O5-C5-C4	3.00	115.10	110.13
7	C	3884	MAN	C1-C2-C3	3.01	113.20	109.55
6	E	3072	BMA	C3-C4-C5	3.03	115.62	110.23
5	G	3716	NAG	C1-O5-C5	3.04	116.61	112.14
7	G	3074	MAN	O5-C1-C2	3.04	115.76	110.89
7	G	3380	MAN	C1-O5-C5	3.05	116.62	112.14
5	C	3374	NAG	O3-C3-C4	3.05	117.23	110.36
7	C	3377	MAN	O2-C2-C1	3.06	115.36	109.23
7	A	3382	MAN	C1-C2-C3	3.08	113.28	109.55
5	B	3232	NAG	C2-N2-C7	3.16	127.22	123.11
7	G	3379	MAN	C1-O5-C5	3.24	116.90	112.14
7	A	3382	MAN	O5-C1-C2	3.26	116.10	110.89
7	C	3378	MAN	C1-O5-C5	3.28	116.96	112.14
7	G	3377	MAN	C1-O5-C5	3.34	117.05	112.14
7	A	3376	MAN	C1-C2-C3	3.34	113.60	109.55
5	F	3190	NAG	C1-O5-C5	3.35	117.06	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	3073	MAN	O5-C1-C2	3.46	116.43	110.89
5	C	3071	NAG	C2-N2-C7	3.51	127.68	123.11
7	A	3073	MAN	C1-O5-C5	3.56	117.37	112.14
7	A	3379	MAN	C1-C2-C3	3.57	113.87	109.55
6	E	3718	BMA	C1-O5-C5	3.59	117.41	112.14
7	C	3719	MAN	O3-C3-C2	3.62	116.65	110.01
5	C	3678	NAG	C1-O5-C5	3.64	117.49	112.14
5	G	3717	NAG	C2-N2-C7	3.67	127.88	123.11
7	C	3719	MAN	C1-O5-C5	3.73	117.63	112.14
7	E	3380	MAN	C1-O5-C5	3.90	117.87	112.14
7	G	3884	MAN	C1-O5-C5	3.91	117.89	112.14
5	E	3678	NAG	C1-O5-C5	3.93	117.92	112.14
7	C	3380	MAN	C1-O5-C5	3.97	117.98	112.14
6	E	3882	BMA	O5-C5-C6	4.01	115.93	107.34
5	H	3232	NAG	C1-O5-C5	4.13	118.21	112.14
5	C	3374	NAG	C2-N2-C7	4.38	128.81	123.11
5	C	3880	NAG	C2-N2-C7	4.42	128.85	123.11
7	A	3382	MAN	C1-O5-C5	4.47	118.71	112.14
7	C	3883	MAN	O5-C1-C2	4.48	118.06	110.89
7	G	3376	MAN	O3-C3-C2	4.59	118.42	110.01
7	A	3719	MAN	C1-O5-C5	4.65	118.98	112.14
5	C	3717	NAG	C2-N2-C7	4.67	129.18	123.11
7	A	3379	MAN	C1-O5-C5	5.00	119.50	112.14
6	C	3375	BMA	O3-C3-C2	5.10	119.36	110.01
5	A	3042	NAG	C2-N2-C7	5.18	129.84	123.11
6	E	3072	BMA	O3-C3-C2	5.19	119.52	110.01
7	G	3074	MAN	C1-O5-C5	5.45	120.15	112.14
7	G	3883	MAN	C1-O5-C5	5.51	120.25	112.14
6	A	3375	BMA	C1-O5-C5	5.56	120.32	112.14
7	C	3884	MAN	C1-O5-C5	5.58	120.34	112.14
7	E	3884	MAN	C1-O5-C5	5.89	120.80	112.14
7	G	3073	MAN	C1-O5-C5	6.25	121.34	112.14
7	C	3883	MAN	C1-O5-C5	6.43	121.59	112.14
5	E	3880	NAG	C2-N2-C7	7.16	132.42	123.11
5	G	3881	NAG	C2-N2-C7	7.22	132.50	123.11
5	H	3232	NAG	C2-N2-C7	7.92	133.41	123.11
5	E	3920	NAG	C1-O5-C5	10.17	127.09	112.14
5	E	3920	NAG	C2-N2-C7	10.58	136.87	123.11

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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	3716	NAG	3	0
6	G	3718	BMA	1	0
7	G	3719	MAN	1	0
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

All (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
2	D	416	THR	12.6
1	C	817	GLN	11.5
2	B	433	ASP	10.6
1	C	818	LYS	10.5
2	H	432	ARG	10.5
2	H	92	ALA	10.4
2	D	393	VAL	10.3
2	D	189	THR	9.9
2	D	83	LEU	9.8
2	H	430	GLN	9.7
2	B	430	GLN	9.5

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Mol	Chain	Res	Type	RSRZ
2	F	91	ALA	9.5
2	D	433	ASP	9.4
2	F	92	ALA	8.9
2	H	91	ALA	8.8
2	H	417	VAL	8.7
2	D	207	ASN	8.6
2	D	610	LEU	8.6
2	D	650	VAL	8.2
2	D	97	PHE	8.2
2	B	432	ARG	8.0
1	E	727	PHE	7.9
2	B	431	SER	7.9
2	B	72	GLY	7.8
2	H	416	THR	7.7
1	A	727	PHE	7.7
2	H	80	LYS	7.7
2	D	144	ILE	7.7
2	D	443	LEU	7.6
2	D	105	ILE	7.3
1	G	817	GLN	7.2
2	D	143	ARG	7.2
2	H	434	ARG	7.1
1	C	335	GLU	7.1
2	D	654	LEU	7.0
2	D	206	GLY	6.9
1	C	816	GLY	6.9
2	F	163	ASP	6.9
2	F	176	CYS	6.8
2	D	135	LEU	6.8
1	C	819	GLN	6.7
1	C	397	GLY	6.7
2	D	109	TYR	6.7
2	D	68	ASP	6.7
2	H	321	GLY	6.6
1	G	624	VAL	6.6
1	G	626	SER	6.6
2	F	206	GLY	6.6
2	D	345	VAL	6.6
1	E	102	TYR	6.6
2	H	175	GLU	6.5
2	D	78	PRO	6.5
2	D	415	VAL	6.4

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Mol	Chain	Res	Type	RSRZ
1	C	398	VAL	6.3
2	D	107	LEU	6.2
2	F	160	THR	6.2
2	D	432	ARG	6.2
2	F	81	VAL	6.1
1	C	393	ALA	6.1
1	A	1044	LYS	6.1
1	C	106	LEU	6.0
1	A	10	ALA	6.0
2	D	62	LEU	6.0
2	D	175	GLU	6.0
1	A	817	GLN	5.9
2	B	321	GLY	5.8
1	C	653	GLN	5.8
2	H	469	GLN	5.8
2	B	417	VAL	5.7
1	G	818	LYS	5.7
2	H	470	GLU	5.7
2	B	91	ALA	5.7
2	D	29	PHE	5.7
2	D	603	TYR	5.6
2	D	401	GLU	5.6
1	C	326	SER	5.6
2	H	393	VAL	5.6
2	D	67	GLU	5.6
2	D	63	ALA	5.6
2	D	628	LEU	5.5
2	D	131	LEU	5.4
2	B	144	ILE	5.4
1	C	723	PRO	5.4
2	H	207	ASN	5.4
2	D	384	ASN	5.4
1	C	102	TYR	5.4
2	D	399	ILE	5.4
2	F	629	GLN	5.4
2	H	389	PHE	5.3
2	H	328	SER	5.3
2	D	160	THR	5.3
2	D	417	VAL	5.3
2	D	606	CYS	5.2
2	F	207	ASN	5.2
1	C	485	TRP	5.2

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Mol	Chain	Res	Type	RSRZ
2	D	101	LYS	5.2
2	D	331	VAL	5.2
2	D	408	ALA	5.1
2	F	26	LYS	5.1
2	B	81	VAL	5.1
2	D	208	LEU	5.1
2	F	83	LEU	5.1
2	F	1	GLN	5.1
2	H	452	THR	5.0
1	C	108	PHE	5.0
1	G	326	SER	5.0
1	C	919	LEU	5.0
2	D	1	GLN	5.0
2	D	159	ASN	5.0
2	H	431	SER	5.0
2	D	391	VAL	4.9
1	A	819	GLN	4.9
1	C	1078	LEU	4.9
2	D	363	PHE	4.9
2	D	623	ALA	4.9
2	D	104	PRO	4.9
2	D	390	GLN	4.9
2	B	429	ASP	4.8
2	D	430	GLN	4.8
2	D	626	PRO	4.8
2	H	186	LEU	4.8
2	B	131	LEU	4.8
2	D	378	CYS	4.8
2	D	236	LEU	4.8
2	D	176	CYS	4.8
1	C	1045	VAL	4.8
2	H	206	GLY	4.7
1	E	726	ALA	4.7
2	D	49	ARG	4.7
2	D	651	ALA	4.7
1	C	122	SER	4.7
1	E	129	GLN	4.7
2	D	102	GLY	4.6
2	H	73	GLN	4.6
2	F	385	VAL	4.6
2	F	78	PRO	4.6
2	D	126	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	10	ALA	4.6
1	G	625	VAL	4.6
2	D	625	CYS	4.6
1	C	725	LEU	4.6
2	F	628	LEU	4.5
1	E	40	ALA	4.5
2	H	335	LYS	4.5
2	D	75	GLN	4.5
2	B	127	LEU	4.5
2	D	77	SER	4.5
2	B	415	VAL	4.5
2	F	650	VAL	4.5
1	G	335	GLU	4.5
1	C	419	GLN	4.4
2	D	404	PHE	4.4
1	C	87	LEU	4.4
2	B	80	LYS	4.4
1	E	95	HIS	4.4
2	F	603	TYR	4.4
1	A	726	ALA	4.4
2	H	244	GLY	4.4
2	B	386	PRO	4.3
2	D	667	VAL	4.3
1	G	128	ARG	4.3
1	C	1044	LYS	4.3
2	B	71	GLY	4.3
2	D	406	ILE	4.3
2	D	622	SER	4.2
2	B	416	THR	4.2
2	D	394	THR	4.2
2	F	175	GLU	4.2
2	H	67	GLU	4.2
1	G	108	PHE	4.1
2	H	115	TYR	4.1
2	F	415	VAL	4.1
2	D	94	ASN	4.1
2	D	652	TYR	4.1
2	F	393	VAL	4.1
2	B	203	LEU	4.1
2	H	377	ASP	4.1
2	B	434	ARG	4.1
1	G	724	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	H	126	LYS	4.1
2	B	651	ALA	4.1
2	D	70	ASN	4.1
2	D	369	THR	4.1
1	G	127	PRO	4.1
1	E	1044	LYS	4.0
1	E	591	VAL	4.0
1	E	721	GLY	4.0
2	D	431	SER	4.0
1	E	921	PHE	4.0
2	H	378	CYS	4.0
2	D	627	GLY	4.0
1	C	1	PHE	4.0
2	D	237	LEU	3.9
1	C	424	TRP	3.9
2	D	38	ILE	3.9
2	D	620	ASN	3.9
2	H	379	ASP	3.9
1	E	482	TRP	3.9
2	B	335	LYS	3.9
1	C	724	LEU	3.9
1	C	593	LEU	3.9
2	H	81	VAL	3.9
2	F	39	ARG	3.9
1	C	726	ALA	3.9
2	H	415	VAL	3.9
2	H	69	HIS	3.9
2	B	145	GLY	3.9
2	D	470	GLU	3.9
1	E	1077	VAL	3.9
2	D	81	VAL	3.8
1	E	817	GLN	3.8
2	D	388	THR	3.8
2	H	442	PHE	3.8
2	D	100	ALA	3.8
1	C	996	GLN	3.8
2	D	370	HIS	3.8
2	B	414	ILE	3.8
2	B	445	CYS	3.8
2	H	423	CYS	3.8
2	B	389	PHE	3.8
2	D	621	CYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	920	ASN	3.7
2	B	83	LEU	3.7
2	B	111	MET	3.7
1	E	41	ALA	3.7
2	B	628	LEU	3.7
2	F	329	ASN	3.7
2	B	97	PHE	3.7
1	E	108	PHE	3.7
2	F	118	LEU	3.7
2	H	327	SER	3.7
2	D	395	ALA	3.7
2	D	65	THR	3.7
2	B	67	GLU	3.7
2	B	206	GLY	3.7
2	H	32	PRO	3.7
2	F	429	ASP	3.7
2	D	56	ILE	3.6
2	F	423	CYS	3.6
2	B	26	LYS	3.6
2	D	74	LYS	3.6
2	D	142	GLY	3.6
2	D	318	SER	3.6
2	B	305	VAL	3.6
2	H	366	ASN	3.6
2	H	333	LEU	3.6
2	D	84	TYR	3.6
2	D	72	GLY	3.6
2	B	69	HIS	3.6
2	F	619	LYS	3.6
2	H	391	VAL	3.6
1	C	48	TYR	3.6
1	C	9	THR	3.6
2	H	93	PHE	3.6
2	F	186	LEU	3.6
2	H	26	LYS	3.6
2	H	243	ASP	3.6
1	E	10	ALA	3.6
1	E	395	TRP	3.6
2	H	376	GLY	3.6
1	C	483	ARG	3.5
1	G	623	GLN	3.5
2	D	602	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	665	ILE	3.5
2	D	365	SER	3.5
2	D	7	LYS	3.5
1	C	721	GLY	3.5
2	D	386	PRO	3.5
1	G	651	ASP	3.5
2	D	382	GLN	3.5
2	F	142	GLY	3.5
2	B	385	VAL	3.5
1	E	9	THR	3.5
2	B	124	VAL	3.5
2	H	174	LYS	3.5
2	H	382	GLN	3.4
2	F	80	LYS	3.4
1	G	1039	GLN	3.4
2	D	419	VAL	3.4
2	D	611	LYS	3.4
2	F	74	LYS	3.4
2	D	330	VAL	3.4
2	D	372	ASN	3.4
2	D	98	ARG	3.4
2	F	406	ILE	3.4
2	D	649	TRP	3.4
1	C	731	ARG	3.4
2	B	404	PHE	3.4
2	D	358	VAL	3.3
2	F	103	TYR	3.3
2	H	50	GLY	3.3
1	G	409	GLN	3.3
2	D	366	ASN	3.3
1	C	400	SER	3.3
1	C	1040	ILE	3.3
2	B	571	ARG	3.3
1	A	621	ARG	3.3
1	C	109	LEU	3.3
1	G	95	HIS	3.3
2	D	414	ILE	3.3
2	D	138	ILE	3.3
1	E	48	TYR	3.3
1	G	433	THR	3.3
2	B	126	LYS	3.3
2	B	93	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	446	GLY	3.3
2	B	50	GLY	3.2
2	D	377	ASP	3.2
2	F	663	TYR	3.2
2	H	298	PHE	3.2
2	H	82	THR	3.2
1	C	730	LEU	3.2
1	E	11	PHE	3.2
1	C	41	ALA	3.2
1	E	592	LEU	3.2
2	H	320	VAL	3.2
2	D	613	GLU	3.2
2	D	30	THR	3.2
1	C	105	GLY	3.2
1	C	104	THR	3.2
2	D	79	GLN	3.2
2	D	210	ALA	3.1
1	G	819	GLN	3.1
2	D	193	ASN	3.1
2	B	133	ARG	3.1
2	H	30	THR	3.1
1	E	1078	LEU	3.1
1	G	919	LEU	3.1
1	A	818	LYS	3.1
1	C	997	LYS	3.1
1	E	335	GLU	3.1
2	B	419	VAL	3.1
2	D	320	VAL	3.1
2	F	330	VAL	3.1
2	D	381	VAL	3.1
2	D	616	PRO	3.1
2	H	654	LEU	3.1
2	F	188	LEU	3.1
2	F	49	ARG	3.1
2	F	664	LEU	3.1
1	G	102	TYR	3.1
2	D	294	ILE	3.1
2	D	95	VAL	3.1
2	D	506	LEU	3.1
1	E	106	LEU	3.0
1	A	816	GLY	3.0
2	F	107	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	161	HIS	3.0
2	F	345	VAL	3.0
2	F	236	LEU	3.0
1	C	722	LYS	3.0
1	E	326	SER	3.0
2	B	413	ASP	3.0
2	H	34	ASP	3.0
2	D	355	THR	3.0
2	H	83	LEU	3.0
2	F	177	GLN	3.0
2	H	404	PHE	3.0
2	D	352	LEU	3.0
2	B	338	TYR	3.0
2	B	664	LEU	3.0
1	E	730	LEU	3.0
2	B	423	CYS	3.0
2	H	173	GLU	3.0
1	A	594	LEU	2.9
2	B	238	VAL	2.9
2	D	624	ALA	2.9
2	H	628	LEU	2.9
2	F	622	SER	2.9
2	B	25	GLN	2.9
2	D	69	HIS	2.9
2	D	71	GLY	2.9
1	E	594	LEU	2.9
2	D	99	ARG	2.9
2	B	38	ILE	2.9
2	H	381	VAL	2.9
2	D	618	GLY	2.9
2	D	182	PHE	2.9
1	E	96	GLU	2.9
2	H	395	ALA	2.9
2	D	39	ARG	2.9
2	F	122	ARG	2.9
2	H	39	ARG	2.9
1	A	592	LEU	2.9
1	A	265	TYR	2.9
2	B	180	PHE	2.9
2	H	84	TYR	2.9
2	B	39	ARG	2.9
2	D	387	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	436	GLY	2.9
1	G	372	ILE	2.9
2	H	429	ASP	2.9
1	G	436	GLY	2.9
2	B	107	LEU	2.9
2	F	384	ASN	2.9
1	E	393	ALA	2.9
2	D	472	GLU	2.9
2	H	122	ARG	2.8
2	D	362	SER	2.8
2	B	376	GLY	2.8
2	D	249	GLY	2.8
2	D	235	ARG	2.8
2	H	363	PHE	2.8
1	A	220	LEU	2.8
1	C	1001	LEU	2.8
2	D	389	PHE	2.8
2	H	56	ILE	2.8
1	C	344	ASP	2.8
1	E	826	HIS	2.8
1	C	482	TRP	2.8
1	C	1028	LEU	2.8
1	C	129	GLN	2.8
2	D	617	PHE	2.8
2	H	463	THR	2.8
2	F	386	PRO	2.8
1	C	345	GLY	2.8
1	C	487	CYS	2.8
1	E	1040	ILE	2.8
2	D	523	ASN	2.8
2	H	629	GLN	2.7
1	C	101	MET	2.7
1	C	65	PRO	2.7
2	D	179	PRO	2.7
2	F	178	PRO	2.7
2	F	119	ASP	2.7
1	A	724	LEU	2.7
2	D	80	LYS	2.7
1	C	814	ALA	2.7
2	H	435	SER	2.7
1	E	38	ILE	2.7
2	D	635	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	729	ASN	2.7
2	H	367	GLY	2.7
1	A	276	ARG	2.7
2	D	139	THR	2.7
2	F	199	VAL	2.7
2	D	334	ILE	2.7
1	C	110	LEU	2.7
2	D	6	PHE	2.7
1	A	266	ALA	2.7
2	F	144	ILE	2.7
2	D	383	ILE	2.7
2	D	356	LEU	2.7
1	C	1046	SER	2.7
2	D	51	CYS	2.7
2	F	191	ASN	2.7
1	G	553	ILE	2.7
2	B	113	LEU	2.7
2	F	660	MET	2.7
2	D	186	LEU	2.6
2	D	96	THR	2.6
2	D	418	GLN	2.6
2	F	417	VAL	2.6
2	D	248	ALA	2.6
2	F	113	LEU	2.6
1	A	296	LYS	2.6
1	C	347	VAL	2.6
2	D	619	LYS	2.6
2	D	428	ARG	2.6
1	G	820	GLY	2.6
2	H	401	GLU	2.6
1	E	37	LYS	2.6
2	H	111	MET	2.6
2	H	664	LEU	2.6
1	E	920	ASN	2.6
2	H	339	ASN	2.6
1	C	121	VAL	2.6
1	C	702	SER	2.6
1	C	443	LEU	2.6
1	C	467	GLN	2.6
2	F	626	PRO	2.6
2	D	376	GLY	2.6
2	F	8	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	84	TYR	2.6
2	H	263	ARG	2.6
2	D	8	VAL	2.6
1	A	623	GLN	2.6
1	G	594	LEU	2.6
2	F	266	LEU	2.6
2	H	38	ILE	2.6
1	C	11	PHE	2.6
2	D	353	PRO	2.6
1	C	565	PHE	2.6
1	C	863	PHE	2.5
1	A	918	TYR	2.5
2	F	624	ALA	2.5
2	F	652	TYR	2.5
2	D	219	MET	2.5
2	F	430	GLN	2.5
2	F	20	GLY	2.5
2	D	57	MET	2.5
2	F	618	GLY	2.5
2	D	180	PHE	2.5
2	B	66	GLN	2.5
2	D	646	GLU	2.5
2	F	321	GLY	2.5
1	A	1080	LYS	2.5
2	F	111	MET	2.5
2	F	193	ASN	2.5
1	C	964	TRP	2.5
1	E	1076	THR	2.5
2	B	96	THR	2.5
2	H	330	VAL	2.5
2	H	665	ILE	2.5
2	D	174	LYS	2.5
2	D	409	LEU	2.5
2	H	203	LEU	2.5
2	F	642	GLU	2.5
2	F	377	ASP	2.5
2	F	616	PRO	2.5
2	H	150	VAL	2.5
2	B	464	GLN	2.5
1	C	596	THR	2.5
2	B	29	PHE	2.5
1	C	401	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	413	ASP	2.5
2	D	643	ARG	2.5
2	B	101	LYS	2.5
2	H	358	VAL	2.5
2	D	250	ASP	2.5
2	H	297	ILE	2.5
2	B	372	ASN	2.5
2	H	630	LEU	2.5
2	F	232	ASN	2.5
1	E	339	ALA	2.5
1	C	409	GLN	2.5
2	D	407	ARG	2.5
1	E	887	THR	2.4
2	H	464	GLN	2.4
1	A	1028	LEU	2.4
2	F	131	LEU	2.4
2	B	603	TYR	2.4
2	H	170	PRO	2.4
1	C	992	LEU	2.4
2	F	29	PHE	2.4
1	A	280	LYS	2.4
2	D	150	VAL	2.4
2	D	108	TYR	2.4
1	A	1078	LEU	2.4
2	H	236	LEU	2.4
2	H	319	ALA	2.4
1	C	553	ILE	2.4
2	B	454	TYR	2.4
2	D	93	PHE	2.4
1	A	323	THR	2.4
1	A	887	THR	2.4
2	F	416	THR	2.4
1	A	485	TRP	2.4
2	B	49	ARG	2.4
1	E	653	GLN	2.4
2	F	632	ASN	2.4
2	F	347	LEU	2.4
2	D	367	GLY	2.4
2	H	249	GLY	2.4
1	C	918	TYR	2.4
2	F	210	ALA	2.4
2	H	144	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	106	LEU	2.4
1	A	1045	VAL	2.3
2	D	209	ASP	2.3
2	D	76	LEU	2.3
2	D	642	GLU	2.3
1	E	992	LEU	2.3
2	F	635	VAL	2.3
1	C	1076	THR	2.3
1	A	273	PHE	2.3
1	A	335	GLU	2.3
2	D	234	THR	2.3
2	D	434	ARG	2.3
1	C	86	LEU	2.3
1	C	592	LEU	2.3
2	H	406	ILE	2.3
1	C	1018	PHE	2.3
1	G	627	GLU	2.3
1	E	39	THR	2.3
2	D	45	GLN	2.3
1	E	372	ILE	2.3
2	D	360	TYR	2.3
1	E	93	VAL	2.3
1	G	437	SER	2.3
2	H	386	PRO	2.3
1	E	627	GLU	2.3
1	A	959	ASN	2.3
2	H	414	ILE	2.3
2	D	321	GLY	2.3
1	E	101	MET	2.3
1	E	52	TYR	2.3
2	H	95	VAL	2.3
2	F	174	LYS	2.3
2	D	561	LEU	2.3
2	F	40	CYS	2.3
1	A	863	PHE	2.3
1	A	436	GLY	2.3
1	C	1041	LEU	2.3
1	E	590	GLN	2.3
2	D	614	LYS	2.3
2	H	603	TYR	2.3
2	B	463	THR	2.3
2	F	638	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	627	GLU	2.2
2	H	124	VAL	2.2
2	H	273	ARG	2.2
2	D	364	CYS	2.2
2	D	368	VAL	2.2
2	D	222	ALA	2.2
2	H	308	TYR	2.2
2	B	34	ASP	2.2
1	C	703	CYS	2.2
1	C	939	ASN	2.2
1	C	1077	VAL	2.2
1	E	1045	VAL	2.2
2	F	665	ILE	2.2
2	H	187	LYS	2.2
2	H	205	SER	2.2
1	G	650	ARG	2.2
2	D	278	ASP	2.2
2	H	65	THR	2.2
2	F	630	LEU	2.2
2	F	38	ILE	2.2
1	E	981	SER	2.2
2	D	400	GLN	2.2
2	D	429	ASP	2.2
1	G	595	ARG	2.2
2	D	115	TYR	2.2
1	C	969	VAL	2.2
1	E	1036	TRP	2.2
1	C	774	LEU	2.2
1	C	904	ALA	2.2
1	G	362	LEU	2.2
1	G	1066	GLN	2.2
2	B	207	ASN	2.2
2	D	28	ASN	2.2
1	E	33	GLY	2.2
1	C	56	ALA	2.2
2	H	131	LEU	2.2
2	H	316	PRO	2.2
1	C	1047	VAL	2.2
2	D	251	GLY	2.2
2	B	285	LEU	2.1
1	A	653	GLN	2.1
1	G	863	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	104	PRO	2.1
2	D	111	MET	2.1
2	B	82	THR	2.1
2	B	652	TYR	2.1
2	F	84	TYR	2.1
1	A	267	ILE	2.1
2	B	401	GLU	2.1
1	G	397	GLY	2.1
1	A	277	ASN	2.1
1	C	499	TRP	2.1
1	C	952	PHE	2.1
2	F	649	TRP	2.1
1	C	125	GLU	2.1
1	C	402	VAL	2.1
1	G	562	LEU	2.1
1	E	100	ASN	2.1
1	E	565	PHE	2.1
2	F	63	ALA	2.1
2	H	419	VAL	2.1
2	D	423	CYS	2.1
2	F	414	ILE	2.1
1	A	322	THR	2.1
2	D	402	GLN	2.1
2	H	189	THR	2.1
2	D	671	ARG	2.1
1	C	421	SER	2.1
2	D	158	VAL	2.1
1	C	732	PRO	2.1
2	H	271	TYR	2.1
2	H	337	ALA	2.1
1	A	234	ILE	2.1
1	C	383	ASP	2.1
1	G	396	LYS	2.1
2	B	183	ARG	2.1
1	C	974	ASN	2.1
2	B	109	TYR	2.1
1	A	626	SER	2.1
2	F	126	LYS	2.1
2	F	398	CYS	2.1
1	C	417	PHE	2.1
2	B	122	ARG	2.1
2	H	248	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	136	LEU	2.1
1	E	485	TRP	2.1
2	D	260	ASN	2.1
2	B	331	VAL	2.1
2	F	138	ILE	2.1
2	H	202	GLN	2.0
2	B	320	VAL	2.0
1	A	106	LEU	2.0
1	G	653	GLN	2.0
2	B	337	ALA	2.0
2	D	136	ASN	2.0
2	D	106	ASP	2.0
2	F	390	GLN	2.0
2	H	326	ASP	2.0
2	D	319	ALA	2.0
2	F	165	LEU	2.0
1	A	221	PHE	2.0
1	G	424	TRP	2.0
2	F	431	SER	2.0
1	E	624	VAL	2.0
1	C	820	GLY	2.0
2	B	428	ARG	2.0
1	G	417	PHE	2.0
2	D	612	PHE	2.0
1	C	422	ARG	2.0
2	D	385	VAL	2.0
2	F	124	VAL	2.0
2	H	237	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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

There are no such residues in this entry.