Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 12:38 AM EDT

PDB ID	:	1G9N
Title	:	HIV-1 YU2 GP120 ENVELOPE GLYCOPROTEIN COMPLEXED WITH CD4 AND INDUCED NEUTRALIZING ANTIBODY 17B
Authors	:	Kwong, P.D.; Wyatt, R.; Majeed, S.; Robinson, J.; Sweet, R.W.; Sodroski, J.; Hendrickson, W.A.
Deposited on	:	2000-11-25
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

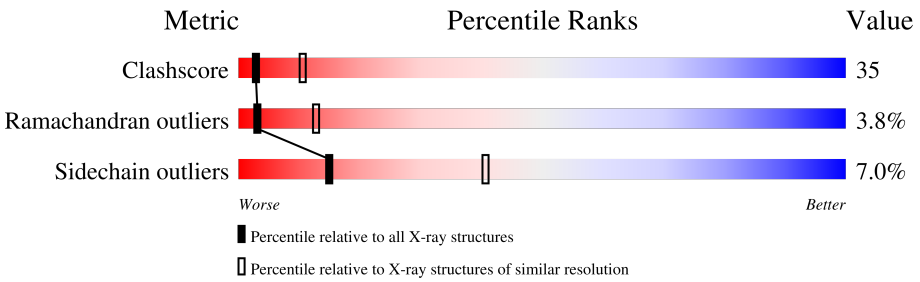
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	G	313	46% 47% · ·
2	C	185	37% 53% 8% ·
3	L	214	41% 52% 7%
4	H	229	43% 50% 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	G	588	X	-	-	-
5	NAG	G	741	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7714 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 ENVELOPE GLYCOPROTEIN GP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	306	2385	1494	417	454	20	1	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	79	GLY	-	cloning artifact	UNP P35961
G	80	ALA	-	cloning artifact	UNP P35961
G	81	ARG	-	cloning artifact	UNP P35961
G	82	SER	-	cloning artifact	UNP P35961
G	128	GLY	-	see remark 999	UNP P35961
G	129	ALA	-	see remark 999	UNP P35961
G	194	GLY	-	see remark 999	UNP P35961
G	298	GLY	-	see remark 999	UNP P35961
G	299	ALA	-	see remark 999	UNP P35961
G	329	GLY	-	see remark 999	UNP P35961

- Molecule 2 is a protein called T-CELL SURFACE GLYCOPROTEIN CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	181	1412	885	247	276	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	184	ASN	SER	engineered mutation	UNP P01730
C	185	THR	ILE	engineered mutation	UNP P01730

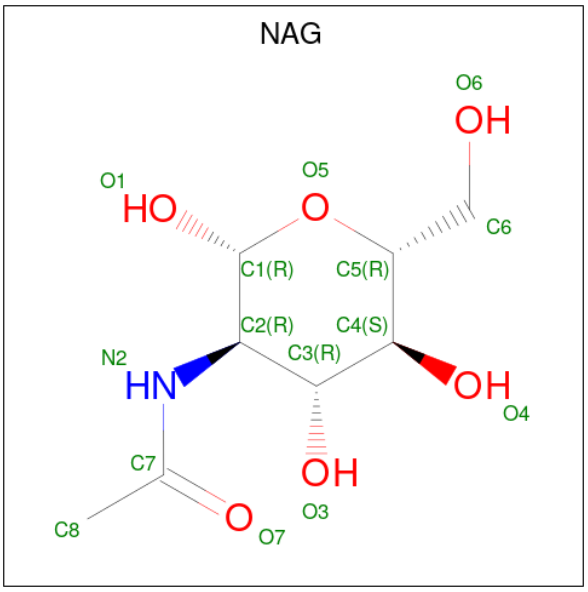
- Molecule 3 is a protein called ANTIBODY 17B, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	214	1650	1032	283	331	4	0	0	0

- Molecule 4 is a protein called ANTIBODY 17B, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	229	1726	1090	294	337	5	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	G	133	133	133	0	0
			Total	O		
6	C	59	59	59	0	0
			Total	O		
6	L	67	67	67	0	0
			Total	O		
6	H	86	86	86	0	0

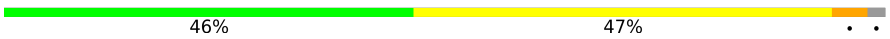
3 Residue-property plots (i)

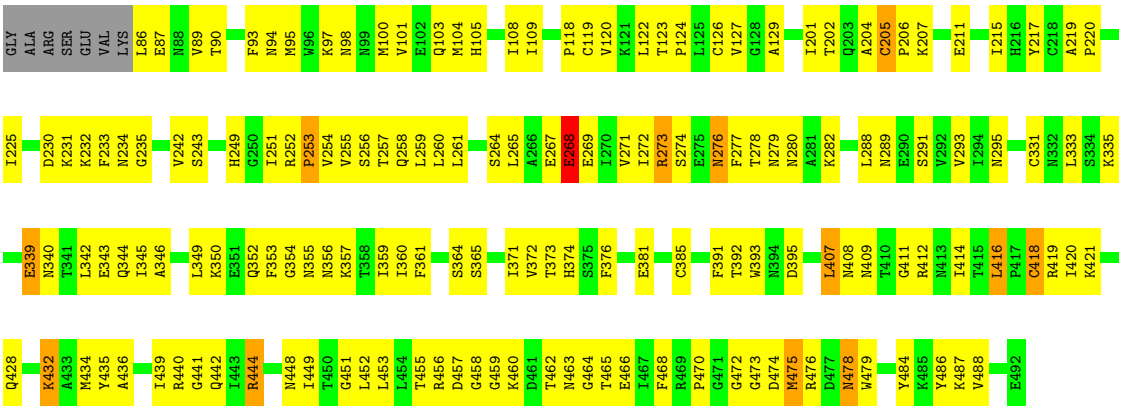
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: ENVELOPE GLYCOPROTEIN GP120

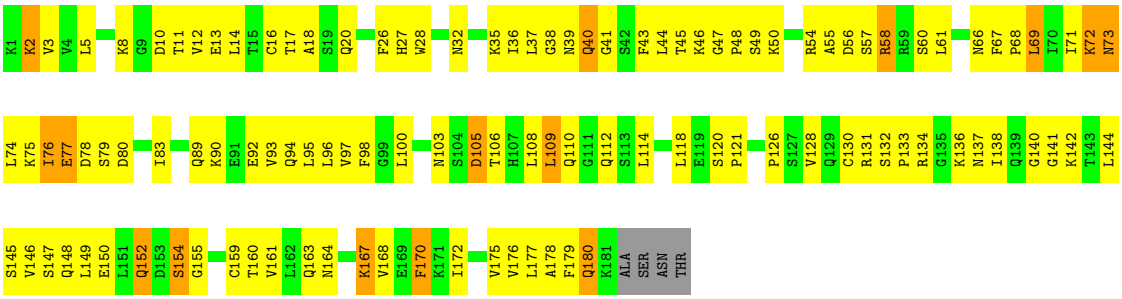
Chain G:





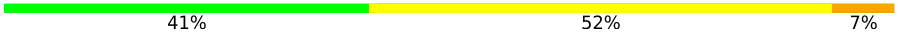
• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD4

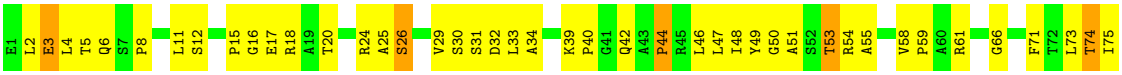
Chain C:

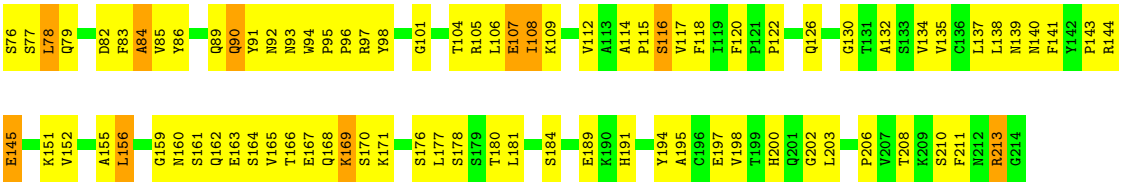


• Molecule 3: ANTIBODY 17B, LIGHT CHAIN

Chain L:

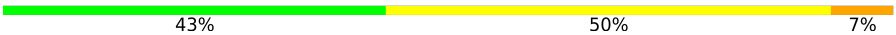


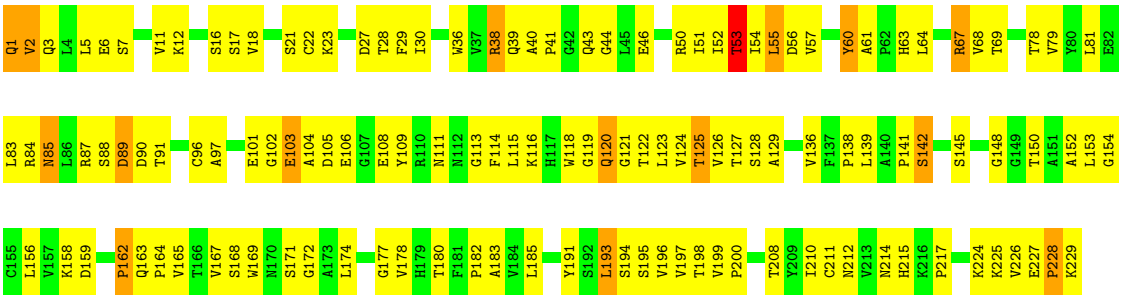




• Molecule 4: ANTIBODY 17B, HEAVY CHAIN

Chain H:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	174.98Å 81.71Å 74.48Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	96.8 (20.00-2.90)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7714	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	G	0.46	0/2432	0.63	0/3296
2	C	0.37	0/1432	0.56	0/1930
3	L	0.38	0/1687	0.57	0/2292
4	H	0.43	0/1766	0.60	0/2405
All	All	0.42	0/7317	0.60	0/9923

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	G	2385	0	2327	165	0
2	C	1412	0	1444	110	0
3	L	1650	0	1603	136	0
4	H	1726	0	1708	125	0
5	G	196	0	182	15	0
6	C	59	0	0	8	0
6	G	133	0	0	11	0
6	H	86	0	0	10	0
6	L	67	0	0	8	0
All	All	7714	0	7264	512	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (512) 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)
3:L:46:LEU:HD12	4:H:116:LYS:HA	1.40	1.00
3:L:97:ARG:HD3	6:L:242:HOH:O	1.62	0.98
2:C:140:GLY:HA3	2:C:144:LEU:HG	1.48	0.95
2:C:130:CYS:HA	2:C:159:CYS:HA	1.50	0.92
1:G:280:ASN:HD22	1:G:458:GLY:H	1.18	0.91
2:C:108:LEU:HD21	2:C:112:GLN:HB3	1.53	0.90
1:G:95:MET:HE2	1:G:235:GLY:HA3	1.55	0.88
2:C:58:ARG:HD2	6:C:191:HOH:O	1.71	0.88
4:H:57:VAL:HA	6:H:286:HOH:O	1.75	0.85
4:H:142:SER:HB3	4:H:145:SER:HB2	1.57	0.85
4:H:210:ILE:HG12	4:H:225:LYS:HA	1.57	0.85
3:L:78:LEU:HD11	3:L:106:LEU:HD21	1.58	0.83
3:L:94:TRP:CZ3	3:L:96:PRO:HG3	2.13	0.83
2:C:134:ARG:HE	2:C:152:GLN:HB2	1.43	0.83
2:C:150:GLU:HB3	2:C:152:GLN:HE22	1.44	0.82
4:H:178:VAL:HG12	4:H:197:VAL:HB	1.62	0.82
1:G:122:LEU:HD11	4:H:55:LEU:HG	1.61	0.82
3:L:169:LYS:HG3	3:L:170:SER:H	1.47	0.80
1:G:373:THR:HA	6:G:967:HOH:O	1.80	0.79
2:C:150:GLU:HB3	2:C:152:GLN:NE2	1.98	0.77
1:G:202:THR:HG22	3:L:95:PRO:HG3	1.65	0.77
1:G:230:ASP:HB2	6:G:1040:HOH:O	1.84	0.76
2:C:50:LYS:O	2:C:50:LYS:HG2	1.85	0.76
3:L:49:TYR:O	3:L:53:THR:HG23	1.85	0.76
2:C:128:VAL:HB	2:C:144:LEU:HD11	1.67	0.76
4:H:150:THR:HA	4:H:200:PRO:HA	1.68	0.76
3:L:79:GLN:HB3	6:L:245:HOH:O	1.86	0.75
2:C:154:SER:HB2	2:C:176:VAL:H	1.52	0.75
2:C:3:VAL:HG22	2:C:94:GLN:HB3	1.69	0.74
1:G:440:ARG:HD2	1:G:442:GLN:O	1.88	0.73
2:C:77:GLU:CD	2:C:77:GLU:H	1.92	0.72
3:L:32:ASP:HB2	3:L:92:ASN:HB2	1.70	0.72
3:L:46:LEU:HD12	4:H:116:LYS:CA	2.17	0.72
1:G:253:PRO:HA	6:G:1020:HOH:O	1.88	0.71
1:G:392:THR:HG22	5:G:894:NAG:HN2	1.56	0.71
3:L:91:TYR:HA	3:L:98:TYR:CD1	2.27	0.69
4:H:12:LYS:HE2	4:H:17:SER:O	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:36:ILE:HG22	2:C:37:LEU:HD22	1.74	0.69
3:L:94:TRP:HA	3:L:95:PRO:C	2.13	0.69
1:G:269:GLU:HA	1:G:289:ASN:ND2	2.08	0.68
2:C:178:ALA:HA	6:C:206:HOH:O	1.91	0.68
2:C:132:SER:HB3	2:C:136:LYS:HB2	1.75	0.68
1:G:280:ASN:HD22	1:G:458:GLY:N	1.91	0.68
3:L:200:HIS:H	3:L:203:LEU:HD12	1.58	0.68
3:L:33:LEU:HD22	3:L:89:GLN:O	1.93	0.67
1:G:255:VAL:HG13	1:G:475:MET:SD	2.34	0.67
1:G:264:SER:HB2	6:G:1090:HOH:O	1.94	0.67
3:L:33:LEU:HD13	3:L:34:ALA:N	2.09	0.67
1:G:104:MET:HE2	1:G:215:ILE:HD11	1.77	0.67
2:C:20:GLN:HG3	6:C:231:HOH:O	1.95	0.67
2:C:58:ARG:HG2	2:C:61:LEU:HG	1.75	0.67
1:G:439:ILE:HD12	1:G:440:ARG:N	2.10	0.66
1:G:273:ARG:HG2	1:G:273:ARG:HH11	1.60	0.66
5:G:963:NAG:H82	5:G:963:NAG:H3	1.77	0.66
1:G:95:MET:HE1	1:G:273:ARG:HH11	1.61	0.66
1:G:104:MET:O	1:G:108:ILE:HG12	1.96	0.66
4:H:141:PRO:HG3	4:H:153:LEU:HD13	1.77	0.66
2:C:61:LEU:HB3	2:C:66:ASN:HB3	1.78	0.65
3:L:167:GLU:N	6:L:218:HOH:O	2.29	0.65
1:G:350:LYS:HE2	1:G:359:ILE:HD13	1.79	0.65
1:G:232:LYS:HE3	6:G:1096:HOH:O	1.95	0.65
3:L:118:PHE:CD2	4:H:152:ALA:HB3	2.31	0.65
1:G:353:PHE:CE2	1:G:456:ARG:HD3	2.32	0.65
1:G:419:ARG:NH2	4:H:103:GLU:OE1	2.30	0.65
1:G:278:THR:HG22	5:G:776:NAG:O6	1.97	0.64
3:L:143:PRO:HB2	3:L:145:GLU:OE1	1.97	0.64
4:H:174:LEU:HA	6:H:253:HOH:O	1.97	0.64
1:G:95:MET:CE	1:G:484:TYR:HB2	2.26	0.64
1:G:280:ASN:O	2:C:35:LYS:HD2	1.98	0.64
3:L:108:ILE:HG23	6:L:215:HOH:O	1.97	0.64
3:L:195:ALA:HA	3:L:210:SER:HB3	1.80	0.64
2:C:76:ILE:HD12	2:C:76:ILE:H	1.62	0.63
2:C:83:ILE:HG23	2:C:92:GLU:HG3	1.80	0.63
1:G:463:ASN:O	1:G:465:THR:HG22	1.98	0.63
4:H:50:ARG:CZ	6:H:273:HOH:O	2.46	0.63
2:C:5:LEU:HD22	2:C:96:LEU:HB2	1.79	0.63
1:G:260:LEU:HA	6:G:1043:HOH:O	1.98	0.63
4:H:85:ASN:N	4:H:85:ASN:HD22	1.94	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:131:ARG:CZ	2:C:137:ASN:HB3	2.29	0.62
1:G:412:ARG:HA	5:G:908:NAG:O6	1.98	0.62
2:C:161:VAL:O	2:C:167:LYS:HA	1.99	0.62
3:L:29:VAL:HG13	3:L:92:ASN:HB3	1.81	0.62
1:G:391:PHE:CD2	1:G:470:PRO:HG3	2.34	0.62
3:L:138:LEU:HD22	3:L:177:LEU:HD23	1.81	0.61
3:L:145:GLU:OE1	3:L:145:GLU:N	2.33	0.61
4:H:165:VAL:HG23	4:H:214:ASN:O	2.01	0.61
4:H:1:GLN:HA	6:H:297:HOH:O	1.98	0.61
1:G:295:ASN:HD22	1:G:444:ARG:NH2	1.99	0.61
2:C:126:PRO:HD2	2:C:142:LYS:HE2	1.82	0.61
3:L:12:SER:HB2	3:L:109:LYS:HB2	1.82	0.61
1:G:339:GLU:O	1:G:343:GLU:HG3	2.01	0.61
1:G:104:MET:HA	1:G:217:TYR:OH	2.01	0.61
1:G:487:LYS:O	1:G:487:LYS:HG3	2.00	0.61
4:H:139:LEU:HD11	4:H:156:LEU:HB2	1.82	0.60
4:H:50:ARG:NH2	4:H:101:GLU:OE2	2.30	0.60
2:C:26:PHE:CZ	2:C:67:PHE:HB3	2.37	0.60
3:L:138:LEU:HD22	3:L:177:LEU:HB3	1.83	0.60
1:G:391:PHE:CG	1:G:470:PRO:HG3	2.36	0.60
3:L:137:LEU:HD12	4:H:196:VAL:HG11	1.82	0.60
2:C:133:PRO:HG2	2:C:155:GLY:HA3	1.84	0.60
1:G:269:GLU:HG2	5:G:789:NAG:HN2	1.66	0.60
1:G:254:VAL:HG11	1:G:261:LEU:HB2	1.84	0.59
4:H:67:ARG:O	4:H:83:LEU:HD23	2.03	0.59
1:G:124:PRO:CG	2:C:60:SER:HA	2.31	0.59
2:C:17:THR:HG23	6:C:236:HOH:O	2.01	0.59
2:C:154:SER:OG	2:C:175:VAL:HA	2.03	0.59
3:L:94:TRP:HA	3:L:95:PRO:O	2.01	0.59
4:H:103:GLU:N	4:H:108:GLU:OE2	2.31	0.59
2:C:103:ASN:N	2:C:103:ASN:HD22	2.00	0.59
3:L:122:PRO:HD3	3:L:134:VAL:HG22	1.85	0.59
4:H:38:ARG:HD2	4:H:46:GLU:OE1	2.02	0.59
1:G:452:LEU:N	1:G:452:LEU:HD12	2.16	0.59
1:G:451:GLY:C	1:G:452:LEU:HD12	2.23	0.58
1:G:101:VAL:HG13	1:G:479:TRP:HB2	1.85	0.58
3:L:83:PHE:O	3:L:84:ALA:HB2	2.03	0.58
4:H:104:ALA:HA	4:H:108:GLU:O	2.02	0.58
4:H:97:ALA:HB3	4:H:115:LEU:HD13	1.84	0.58
3:L:107:GLU:HG2	3:L:108:ILE:N	2.18	0.58
1:G:118:PRO:HG3	1:G:435:TYR:CZ	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:28:TRP:HB2	2:C:37:LEU:HD23	1.85	0.58
1:G:242:VAL:HG22	1:G:243:SER:N	2.19	0.58
4:H:178:VAL:HG22	6:H:303:HOH:O	2.03	0.58
2:C:75:LYS:HB3	2:C:77:GLU:OE1	2.02	0.58
3:L:115:PRO:HD2	3:L:203:LEU:HG	1.85	0.58
4:H:169:TRP:HB2	4:H:174:LEU:O	2.04	0.58
3:L:91:TYR:HB2	4:H:113:GLY:HA3	1.86	0.57
1:G:100:MET:HE1	1:G:487:LYS:N	2.19	0.57
3:L:93:ASN:ND2	3:L:97:ARG:HB2	2.19	0.57
1:G:288:LEU:HD21	1:G:345:ILE:HD11	1.85	0.57
1:G:365:SER:HB2	2:C:46:LYS:O	2.04	0.57
4:H:12:LYS:O	4:H:126:VAL:HA	2.04	0.57
4:H:197:VAL:HG22	4:H:199:VAL:HG13	1.85	0.57
3:L:4:LEU:HD13	3:L:25:ALA:HB2	1.85	0.57
3:L:29:VAL:O	3:L:29:VAL:HG12	2.04	0.57
1:G:371:ILE:HG21	2:C:45:THR:HG22	1.86	0.57
4:H:36:TRP:CE2	4:H:81:LEU:HB2	2.40	0.57
4:H:6:GLU:OE2	4:H:121:GLY:N	2.36	0.56
1:G:87:GLU:HG2	1:G:89:VAL:HG12	1.87	0.56
1:G:256:SER:HB2	1:G:376:PHE:HB3	1.86	0.56
1:G:288:LEU:HD12	1:G:449:ILE:O	2.05	0.56
1:G:456:ARG:HB3	1:G:468:PHE:CE2	2.41	0.56
2:C:16:CYS:HB2	2:C:28:TRP:CZ2	2.41	0.56
3:L:20:THR:HG23	3:L:74:THR:HG23	1.87	0.56
4:H:51:ILE:HG23	4:H:51:ILE:O	2.06	0.56
2:C:54:ARG:O	2:C:72:LYS:NZ	2.35	0.56
3:L:108:ILE:HG13	3:L:168:GLN:HG2	1.87	0.56
3:L:151:LYS:HE2	3:L:156:LEU:HD23	1.87	0.56
1:G:353:PHE:CZ	1:G:456:ARG:HD3	2.41	0.56
3:L:78:LEU:HD23	3:L:79:GLN:N	2.21	0.55
3:L:189:GLU:HA	3:L:213:ARG:NH1	2.21	0.55
2:C:154:SER:CB	2:C:176:VAL:H	2.18	0.55
2:C:98:PHE:HB3	2:C:118:LEU:HD11	1.88	0.55
3:L:115:PRO:HD3	3:L:200:HIS:ND1	2.21	0.55
1:G:456:ARG:HB3	1:G:468:PHE:CD2	2.42	0.55
2:C:76:ILE:HA	2:C:97:VAL:HB	1.88	0.55
3:L:161:SER:HA	3:L:180:THR:O	2.06	0.55
4:H:85:ASN:N	4:H:85:ASN:ND2	2.55	0.55
1:G:205:CYS:N	1:G:206:PRO:HD3	2.21	0.55
3:L:166:THR:HG22	4:H:182:PRO:HD3	1.88	0.55
2:C:108:LEU:HD23	2:C:109:LEU:N	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:156:LEU:HD13	3:L:156:LEU:O	2.06	0.54
1:G:371:ILE:HD12	1:G:472:GLY:O	2.07	0.54
1:G:204:ALA:C	1:G:206:PRO:HD3	2.28	0.54
1:G:356:ASN:ND2	5:G:856:NAG:H61	2.22	0.54
3:L:141:PHE:HE1	3:L:177:LEU:H	1.55	0.54
2:C:36:ILE:HD13	2:C:49:SER:CB	2.37	0.54
4:H:227:GLU:HG2	4:H:228:PRO:HD2	1.89	0.54
3:L:86:TYR:HE2	3:L:106:LEU:HD22	1.73	0.54
4:H:52:ILE:HG23	4:H:109:TYR:CZ	2.42	0.54
1:G:98:ASN:HB3	1:G:101:VAL:HG23	1.90	0.54
1:G:460:LYS:HB2	2:C:32:ASN:O	2.08	0.54
1:G:87:GLU:H	1:G:243:SER:HA	1.72	0.53
1:G:95:MET:CE	1:G:235:GLY:HA3	2.34	0.53
1:G:215:ILE:HG12	1:G:251:ILE:O	2.09	0.53
2:C:170:PHE:O	2:C:172:ILE:HG12	2.09	0.53
1:G:86:LEU:HA	1:G:243:SER:HB3	1.90	0.53
3:L:165:VAL:HG12	3:L:166:THR:N	2.23	0.53
2:C:2:LYS:HB3	2:C:93:VAL:HG23	1.90	0.53
3:L:2:LEU:HD12	3:L:2:LEU:N	2.24	0.53
1:G:119:CYS:HB2	1:G:434:MET:HE2	1.91	0.53
1:G:373:THR:HB	1:G:385:CYS:O	2.09	0.53
3:L:59:PRO:HB3	3:L:61:ARG:NH1	2.24	0.53
2:C:138:ILE:HD13	2:C:146:VAL:HG22	1.91	0.53
3:L:46:LEU:HD22	3:L:55:ALA:HB2	1.89	0.53
3:L:114:ALA:HB2	3:L:202:GLY:O	2.10	0.52
3:L:135:VAL:HG21	4:H:156:LEU:HD13	1.91	0.52
1:G:392:THR:HG22	1:G:392:THR:O	2.09	0.52
3:L:48:ILE:HG22	3:L:49:TYR:N	2.24	0.52
2:C:83:ILE:HG12	2:C:92:GLU:HG2	1.90	0.52
1:G:100:MET:HE1	1:G:486:TYR:C	2.30	0.52
2:C:128:VAL:HA	2:C:160:THR:O	2.09	0.52
1:G:385:CYS:HA	1:G:418:CYS:HA	1.92	0.52
2:C:83:ILE:HD11	6:C:221:HOH:O	2.09	0.52
4:H:123:LEU:HD12	4:H:124:VAL:H	1.74	0.52
3:L:137:LEU:C	3:L:138:LEU:HD12	2.30	0.52
5:G:697:NAG:H82	5:G:697:NAG:H3	1.92	0.52
2:C:140:GLY:CA	2:C:144:LEU:HG	2.30	0.52
1:G:456:ARG:HD2	1:G:468:PHE:CZ	2.45	0.51
1:G:120:VAL:CG1	1:G:434:MET:HB3	2.40	0.51
3:L:137:LEU:HD23	3:L:138:LEU:N	2.25	0.51
3:L:138:LEU:HB2	3:L:177:LEU:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:102:GLY:O	4:H:104:ALA:N	2.37	0.51
4:H:27:ASP:CG	4:H:28:THR:H	2.12	0.51
4:H:127:THR:HG22	4:H:128:SER:N	2.24	0.51
4:H:163:GLN:HE22	4:H:183:ALA:HB3	1.75	0.51
3:L:48:ILE:HD13	3:L:54:ARG:HA	1.91	0.51
3:L:120:PHE:CD2	4:H:139:LEU:HD23	2.45	0.51
3:L:163:GLU:HB3	3:L:177:LEU:HD11	1.93	0.51
2:C:69:LEU:C	2:C:69:LEU:HD22	2.31	0.51
1:G:219:ALA:HB2	1:G:225:ILE:HG13	1.93	0.51
3:L:73:LEU:HD13	3:L:73:LEU:O	2.11	0.51
1:G:109:ILE:HG23	1:G:428:GLN:HG2	1.93	0.51
4:H:141:PRO:HG3	4:H:153:LEU:CB	2.40	0.51
1:G:273:ARG:HG2	1:G:273:ARG:NH1	2.25	0.51
4:H:68:VAL:HG22	4:H:69:THR:N	2.26	0.51
4:H:148:GLY:HA2	6:H:311:HOH:O	2.11	0.51
1:G:459:GLY:HA3	6:G:1012:HOH:O	2.09	0.50
4:H:127:THR:HG22	4:H:129:ALA:H	1.76	0.50
3:L:18:ARG:HG3	3:L:75:ILE:O	2.10	0.50
3:L:46:LEU:HD13	4:H:116:LYS:HD2	1.93	0.50
4:H:123:LEU:HD12	4:H:124:VAL:N	2.26	0.50
4:H:1:GLN:HG2	4:H:3:GLN:HE22	1.76	0.50
2:C:83:ILE:HA	2:C:92:GLU:HA	1.92	0.50
3:L:50:GLY:O	3:L:51:ALA:HB3	2.12	0.50
4:H:227:GLU:OE1	4:H:229:LYS:HB2	2.12	0.50
1:G:474:ASP:O	1:G:476:ARG:N	2.44	0.50
3:L:11:LEU:HD23	3:L:106:LEU:HD12	1.93	0.50
4:H:40:ALA:HB1	4:H:41:PRO:HD2	1.94	0.50
4:H:40:ALA:HB3	4:H:43:GLN:HG3	1.94	0.50
4:H:91:THR:HG23	4:H:125:THR:HA	1.94	0.50
1:G:360:ILE:HG22	1:G:361:PHE:N	2.26	0.50
4:H:39:GLN:HE21	4:H:44:GLY:HA2	1.76	0.50
1:G:381:GLU:HB3	1:G:420:ILE:HD13	1.93	0.50
3:L:16:GLY:O	3:L:77:SER:HA	2.12	0.50
3:L:165:VAL:HG12	3:L:166:THR:H	1.77	0.50
3:L:195:ALA:CA	3:L:210:SER:HB3	2.42	0.50
4:H:174:LEU:HD21	4:H:199:VAL:HG11	1.92	0.50
1:G:359:ILE:O	1:G:395:ASP:HB2	2.12	0.49
3:L:177:LEU:HD12	3:L:178:SER:H	1.77	0.49
4:H:156:LEU:HD12	4:H:194:SER:OG	2.12	0.49
1:G:124:PRO:HG2	2:C:60:SER:HA	1.95	0.49
1:G:339:GLU:HG3	6:G:1088:HOH:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:66:GLY:HA3	3:L:71:PHE:HA	1.92	0.49
4:H:16:SER:OG	4:H:17:SER:N	2.45	0.49
1:G:276:ASN:OD1	1:G:278:THR:HB	2.13	0.49
3:L:2:LEU:HD23	3:L:29:VAL:HG22	1.93	0.49
3:L:3:GLU:HB3	3:L:26:SER:OG	2.13	0.49
4:H:60:TYR:CE2	4:H:69:THR:HA	2.47	0.49
4:H:169:TRP:CZ2	4:H:211:CYS:HB3	2.46	0.49
1:G:335:LYS:O	1:G:339:GLU:HB2	2.12	0.49
2:C:36:ILE:HA	2:C:49:SER:HB3	1.94	0.49
2:C:28:TRP:CE2	2:C:69:LEU:HB2	2.48	0.49
4:H:2:VAL:HG13	4:H:27:ASP:HB3	1.94	0.49
1:G:421:LYS:HE2	4:H:106:GLU:O	2.12	0.49
3:L:8:PRO:O	3:L:104:THR:HG23	2.13	0.49
3:L:169:LYS:HG3	3:L:170:SER:N	2.23	0.49
4:H:152:ALA:HA	4:H:198:THR:HA	1.96	0.48
1:G:119:CYS:O	1:G:202:THR:HG23	2.14	0.48
1:G:343:GLU:C	1:G:345:ILE:H	2.17	0.48
1:G:459:GLY:O	1:G:462:THR:HG23	2.13	0.48
2:C:76:ILE:H	2:C:76:ILE:CD1	2.23	0.48
2:C:114:LEU:O	2:C:145:SER:HA	2.13	0.48
3:L:191:HIS:HB2	3:L:194:TYR:OH	2.14	0.48
1:G:215:ILE:O	1:G:215:ILE:HG13	2.13	0.48
1:G:457:ASP:HB3	2:C:48:PRO:HG2	1.94	0.48
2:C:36:ILE:HD13	2:C:49:SER:HB2	1.94	0.48
3:L:16:GLY:HA2	3:L:77:SER:OG	2.12	0.48
3:L:29:VAL:CG1	3:L:90:GLN:HG2	2.43	0.48
1:G:249:HIS:O	1:G:251:ILE:HG13	2.14	0.48
3:L:151:LYS:HA	3:L:155:ALA:O	2.14	0.48
4:H:153:LEU:HD12	4:H:226:VAL:HG11	1.94	0.48
2:C:44:LEU:HD12	2:C:45:THR:N	2.29	0.48
3:L:79:GLN:O	3:L:82:ASP:HB2	2.14	0.48
3:L:137:LEU:C	3:L:137:LEU:HD23	2.34	0.48
3:L:169:LYS:NZ	3:L:169:LYS:HA	2.29	0.48
4:H:183:ALA:HA	4:H:193:LEU:HB3	1.96	0.48
1:G:350:LYS:C	1:G:352:GLN:H	2.17	0.48
4:H:154:GLY:HA2	4:H:169:TRP:CH2	2.49	0.48
1:G:105:HIS:O	1:G:109:ILE:HG13	2.14	0.48
1:G:120:VAL:HA	1:G:201:ILE:O	2.14	0.48
1:G:279:ASN:HD22	1:G:282:LYS:HD3	1.79	0.48
4:H:11:VAL:HG21	4:H:162:PRO:HG3	1.96	0.48
4:H:138:PRO:HD3	4:H:224:LYS:HG2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:ILE:HD12	1:G:253:PRO:CB	2.43	0.48
5:G:734:NAG:H4	6:G:1076:HOH:O	2.13	0.48
4:H:88:SER:HA	4:H:126:VAL:O	2.13	0.48
1:G:95:MET:HE3	1:G:234:ASN:O	2.14	0.47
1:G:371:ILE:HD11	2:C:43:PHE:CD2	2.48	0.47
4:H:6:GLU:HB3	4:H:122:THR:OG1	2.14	0.47
4:H:41:PRO:C	4:H:43:GLN:H	2.15	0.47
3:L:48:ILE:CD1	3:L:54:ARG:HA	2.44	0.47
4:H:12:LYS:HG3	4:H:18:VAL:HB	1.95	0.47
4:H:52:ILE:HG23	4:H:109:TYR:OH	2.15	0.47
3:L:144:ARG:HG3	3:L:165:VAL:HG11	1.96	0.47
1:G:342:LEU:HD13	1:G:393:TRP:HB2	1.97	0.47
4:H:67:ARG:HH11	4:H:67:ARG:HB2	1.79	0.47
1:G:448:ASN:ND2	5:G:948:NAG:H82	2.30	0.47
3:L:44:PRO:HD2	4:H:118:TRP:CE3	2.49	0.47
4:H:5:LEU:O	4:H:22:CYS:HA	2.13	0.47
3:L:33:LEU:HD13	3:L:33:LEU:C	2.35	0.47
4:H:61:ALA:HB3	4:H:64:LEU:HD12	1.97	0.47
4:H:67:ARG:HH22	4:H:90:ASP:CG	2.17	0.47
4:H:148:GLY:HA3	6:H:290:HOH:O	2.13	0.47
3:L:29:VAL:HG11	3:L:90:GLN:HG2	1.97	0.47
2:C:26:PHE:CE1	2:C:39:ASN:HB3	2.49	0.47
1:G:100:MET:HE1	1:G:486:TYR:CB	2.45	0.47
1:G:232:LYS:HG3	1:G:271:VAL:HG22	1.96	0.47
1:G:272:ILE:O	1:G:272:ILE:HG13	2.14	0.47
3:L:46:LEU:CD1	4:H:116:LYS:HA	2.27	0.47
4:H:136:VAL:HG11	4:H:211:CYS:SG	2.55	0.47
4:H:229:LYS:HD3	4:H:229:LYS:C	2.35	0.47
5:G:894:NAG:O3	5:G:894:NAG:H83	2.15	0.46
3:L:30:SER:OG	3:L:31:SER:N	2.48	0.46
3:L:39:LYS:HD2	3:L:84:ALA:HB2	1.98	0.46
3:L:197:GLU:CD	3:L:206:PRO:HB3	2.34	0.46
1:G:86:LEU:HA	1:G:243:SER:CB	2.44	0.46
1:G:478:ASN:N	1:G:478:ASN:HD22	2.13	0.46
2:C:128:VAL:CB	2:C:144:LEU:HD11	2.42	0.46
2:C:163:GLN:HG3	2:C:164:ASN:OD1	2.15	0.46
4:H:141:PRO:HG3	4:H:153:LEU:HB3	1.98	0.46
4:H:168:SER:HB3	4:H:172:GLY:HA2	1.96	0.46
4:H:171:SER:HA	4:H:212:ASN:ND2	2.30	0.46
1:G:95:MET:HB3	1:G:484:TYR:HA	1.97	0.46
1:G:269:GLU:CG	5:G:789:NAG:HN2	2.27	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:78:THR:HG22	4:H:79:VAL:N	2.30	0.46
2:C:3:VAL:HG22	2:C:94:GLN:CB	2.43	0.46
2:C:154:SER:HB2	2:C:176:VAL:HG23	1.97	0.46
4:H:54:ILE:HG23	4:H:55:LEU:N	2.31	0.46
4:H:153:LEU:HD12	4:H:226:VAL:CG1	2.46	0.46
1:G:279:ASN:ND2	1:G:282:LYS:HG2	2.30	0.46
1:G:202:THR:CG2	3:L:95:PRO:HG3	2.41	0.46
4:H:7:SER:HB3	4:H:21:SER:OG	2.15	0.46
1:G:360:ILE:CG2	1:G:361:PHE:N	2.78	0.46
2:C:83:ILE:HG23	2:C:92:GLU:CG	2.45	0.46
2:C:103:ASN:N	2:C:103:ASN:ND2	2.63	0.46
2:C:120:SER:OG	2:C:121:PRO:HD2	2.15	0.46
1:G:119:CYS:HB3	3:L:94:TRP:NE1	2.31	0.46
1:G:231:LYS:HB2	1:G:268:GLU:HB2	1.96	0.46
2:C:57:SER:OG	2:C:58:ARG:N	2.49	0.46
4:H:96:CYS:O	4:H:119:GLY:N	2.45	0.46
2:C:50:LYS:HE3	6:C:224:HOH:O	2.16	0.46
3:L:61:ARG:CZ	3:L:79:GLN:HG3	2.46	0.46
4:H:154:GLY:HA2	4:H:169:TRP:CZ2	2.51	0.46
1:G:335:LYS:HD3	1:G:407:LEU:O	2.16	0.45
2:C:14:LEU:HD21	2:C:95:LEU:HD13	1.98	0.45
3:L:2:LEU:CD2	3:L:29:VAL:HG22	2.46	0.45
3:L:166:THR:HB	6:L:218:HOH:O	2.16	0.45
1:G:233:PHE:CE2	1:G:235:GLY:HA2	2.51	0.45
2:C:39:ASN:ND2	2:C:41:GLY:H	2.14	0.45
4:H:215:HIS:CD2	4:H:217:PRO:HD2	2.51	0.45
4:H:29:PHE:CE2	4:H:53:THR:HG21	2.51	0.45
1:G:346:ALA:O	1:G:350:LYS:HG2	2.17	0.45
3:L:61:ARG:NE	3:L:79:GLN:HG3	2.32	0.45
1:G:265:LEU:HD11	1:G:291:SER:H	1.81	0.45
3:L:151:LYS:HD2	6:L:272:HOH:O	2.16	0.45
3:L:191:HIS:C	3:L:213:ARG:HH21	2.20	0.45
4:H:167:VAL:HG11	4:H:195:SER:HB2	1.99	0.45
1:G:118:PRO:HG3	1:G:435:TYR:CE1	2.51	0.45
1:G:259:LEU:HB2	1:G:374:HIS:CE1	2.52	0.45
1:G:279:ASN:HD22	1:G:282:LYS:HG2	1.82	0.45
1:G:335:LYS:HD3	1:G:408:ASN:HA	1.99	0.45
2:C:75:LYS:N	2:C:78:ASP:OD2	2.47	0.45
4:H:53:THR:O	4:H:56:ASP:N	2.49	0.45
4:H:227:GLU:C	4:H:229:LYS:H	2.20	0.45
1:G:242:VAL:CG2	1:G:243:SER:N	2.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:295:ASN:HD22	1:G:444:ARG:HH22	1.65	0.45
1:G:475:MET:O	1:G:478:ASN:HB2	2.17	0.45
2:C:131:ARG:NH1	2:C:137:ASN:HB3	2.31	0.45
3:L:47:LEU:HD11	3:L:86:TYR:CE1	2.51	0.45
3:L:206:PRO:HD3	6:L:275:HOH:O	2.17	0.45
4:H:1:GLN:O	4:H:1:GLN:NE2	2.49	0.45
4:H:67:ARG:HA	4:H:84:ARG:HH11	1.82	0.45
2:C:146:VAL:O	2:C:147:SER:C	2.55	0.44
3:L:39:LYS:HE2	3:L:83:PHE:O	2.17	0.44
1:G:119:CYS:N	1:G:205:CYS:SG	2.90	0.44
1:G:440:ARG:O	1:G:442:GLN:N	2.50	0.44
2:C:27:HIS:ND1	2:C:38:GLY:HA3	2.32	0.44
4:H:141:PRO:HG3	4:H:153:LEU:CD1	2.44	0.44
4:H:171:SER:HA	4:H:212:ASN:HD21	1.82	0.44
3:L:61:ARG:O	3:L:75:ILE:HA	2.16	0.44
3:L:195:ALA:HB1	3:L:208:THR:HG23	1.99	0.44
1:G:371:ILE:CD1	1:G:473:GLY:HA3	2.46	0.44
1:G:466:GLU:HB3	1:G:468:PHE:CE1	2.53	0.44
3:L:197:GLU:HB2	6:L:272:HOH:O	2.17	0.44
4:H:167:VAL:HG11	4:H:195:SER:CB	2.47	0.44
3:L:116:SER:O	3:L:118:PHE:CD1	2.71	0.44
4:H:163:GLN:OE1	4:H:164:PRO:HA	2.18	0.44
1:G:356:ASN:HD21	5:G:856:NAG:H4	1.83	0.44
3:L:194:TYR:HB2	3:L:211:PHE:CE1	2.53	0.44
4:H:177:GLY:O	4:H:197:VAL:HG23	2.18	0.44
4:H:197:VAL:O	4:H:197:VAL:HG13	2.17	0.44
1:G:252:ARG:O	1:G:254:VAL:N	2.50	0.44
2:C:105:ASP:OD2	2:C:106:THR:N	2.51	0.44
3:L:126:GLN:HE22	3:L:132:ALA:CA	2.31	0.44
4:H:111:ASN:OD1	6:H:273:HOH:O	2.21	0.44
1:G:95:MET:CB	1:G:484:TYR:HA	2.48	0.43
2:C:109:LEU:HG	2:C:110:GLN:H	1.83	0.43
3:L:137:LEU:O	3:L:138:LEU:HD12	2.18	0.43
3:L:197:GLU:OE2	3:L:206:PRO:HB3	2.18	0.43
4:H:158:LYS:HG2	4:H:159:ASP:N	2.32	0.43
2:C:55:ALA:O	2:C:56:ASP:HB2	2.18	0.43
3:L:117:VAL:HG22	3:L:198:VAL:HG21	2.00	0.43
1:G:94:ASN:ND2	1:G:97:LYS:HB3	2.34	0.43
3:L:195:ALA:HA	3:L:210:SER:CB	2.47	0.43
2:C:90:LYS:HD3	6:C:214:HOH:O	2.18	0.43
4:H:120:GLN:HE21	4:H:120:GLN:HB2	1.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:MET:HE1	1:G:273:ARG:NH1	2.29	0.43
1:G:260:LEU:HD21	1:G:453:LEU:HD11	2.00	0.43
4:H:150:THR:HG22	4:H:200:PRO:CA	2.49	0.43
1:G:274:SER:HB3	1:G:277:PHE:CD1	2.54	0.43
1:G:293:VAL:HG23	6:G:1018:HOH:O	2.18	0.43
1:G:349:LEU:HD22	1:G:468:PHE:CE2	2.53	0.43
2:C:79:SER:O	2:C:80:ASP:HB2	2.18	0.43
1:G:95:MET:CE	1:G:273:ARG:HH11	2.31	0.43
1:G:257:THR:O	1:G:258:GLN:HB2	2.19	0.43
6:G:970:HOH:O	2:C:47:GLY:HA2	2.17	0.43
2:C:10:ASP:O	2:C:74:LEU:HB2	2.19	0.43
3:L:83:PHE:O	3:L:84:ALA:CB	2.67	0.43
4:H:30:ILE:CD1	4:H:105:ASP:HB3	2.49	0.43
4:H:50:ARG:NH1	6:H:273:HOH:O	2.50	0.43
4:H:50:ARG:HH12	4:H:52:ILE:HG12	1.83	0.43
4:H:87:ARG:O	4:H:126:VAL:HB	2.19	0.43
1:G:452:LEU:N	1:G:452:LEU:CD1	2.82	0.43
4:H:5:LEU:O	4:H:23:LYS:N	2.49	0.43
2:C:8:LYS:HD2	2:C:76:ILE:HG13	2.00	0.43
3:L:55:ALA:O	3:L:58:VAL:HG23	2.19	0.43
1:G:354:GLY:O	1:G:357:LYS:HB2	2.18	0.42
3:L:5:THR:O	3:L:24:ARG:N	2.50	0.42
3:L:39:LYS:HB2	3:L:42:GLN:OE1	2.19	0.42
3:L:152:VAL:HG13	3:L:194:TYR:CE1	2.53	0.42
1:G:100:MET:HE1	1:G:486:TYR:HB3	2.00	0.42
1:G:124:PRO:CB	2:C:60:SER:HA	2.49	0.42
3:L:195:ALA:CB	3:L:210:SER:HB3	2.49	0.42
2:C:17:THR:HG22	2:C:18:ALA:N	2.34	0.42
3:L:11:LEU:HD23	3:L:106:LEU:CD1	2.49	0.42
3:L:117:VAL:CG2	3:L:198:VAL:HG21	2.48	0.42
3:L:141:PHE:HE1	3:L:176:SER:HA	1.84	0.42
4:H:5:LEU:HB2	4:H:23:LYS:HB3	2.01	0.42
4:H:101:GLU:HA	4:H:101:GLU:OE1	2.20	0.42
2:C:133:PRO:HG2	2:C:155:GLY:CA	2.47	0.42
4:H:180:THR:HA	4:H:195:SER:HA	2.02	0.42
2:C:5:LEU:HB2	2:C:168:VAL:HG13	2.01	0.42
2:C:11:THR:HA	2:C:71:ILE:O	2.19	0.42
2:C:77:GLU:OE2	2:C:77:GLU:N	2.52	0.42
2:C:73:ASN:HD22	2:C:73:ASN:HA	1.67	0.42
2:C:110:GLN:NE2	2:C:178:ALA:HB2	2.34	0.42
3:L:40:PRO:HB3	3:L:167:GLU:OE1	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:LEU:HD21	4:H:57:VAL:HG21	2.01	0.42
1:G:295:ASN:O	1:G:331:CYS:HA	2.20	0.42
3:L:3:GLU:N	3:L:26:SER:OG	2.43	0.42
1:G:89:VAL:HG22	1:G:90:THR:N	2.35	0.42
1:G:274:SER:HB3	1:G:277:PHE:CE1	2.54	0.42
2:C:37:LEU:HD23	2:C:37:LEU:O	2.19	0.42
3:L:59:PRO:HB3	3:L:61:ARG:CZ	2.50	0.42
1:G:364:SER:CB	1:G:372:VAL:HA	2.50	0.41
1:G:472:GLY:O	2:C:40:GLN:HG2	2.20	0.41
2:C:5:LEU:CD2	2:C:96:LEU:HB2	2.49	0.41
3:L:85:VAL:HA	3:L:104:THR:O	2.20	0.41
1:G:97:LYS:O	1:G:97:LYS:HG2	2.21	0.41
1:G:105:HIS:HA	1:G:479:TRP:NE1	2.35	0.41
2:C:110:GLN:HB2	2:C:177:LEU:O	2.19	0.41
3:L:2:LEU:HD23	3:L:29:VAL:CG2	2.49	0.41
3:L:17:GLU:CD	3:L:18:ARG:H	2.22	0.41
3:L:33:LEU:HG	3:L:71:PHE:CG	2.55	0.41
1:G:95:MET:HE2	1:G:484:TYR:HB2	2.01	0.41
3:L:169:LYS:HA	3:L:169:LYS:CE	2.51	0.41
1:G:127:VAL:HG23	1:G:129:ALA:H	1.85	0.41
1:G:268:GLU:HB3	1:G:269:GLU:H	1.48	0.41
1:G:279:ASN:HD22	1:G:282:LYS:CG	2.33	0.41
5:G:762:NAG:O3	5:G:762:NAG:C7	2.68	0.41
2:C:12:VAL:HG22	2:C:13:GLU:N	2.35	0.41
3:L:93:ASN:HD21	3:L:97:ARG:HB2	1.84	0.41
3:L:143:PRO:HB2	3:L:145:GLU:CD	2.40	0.41
1:G:335:LYS:NZ	1:G:411:GLY:HA3	2.36	0.41
2:C:112:GLN:O	2:C:149:LEU:HB2	2.21	0.41
3:L:137:LEU:HD11	4:H:196:VAL:HG21	2.01	0.41
4:H:111:ASN:CG	6:H:273:HOH:O	2.57	0.41
2:C:17:THR:HG22	2:C:18:ALA:O	2.19	0.41
3:L:138:LEU:O	3:L:176:SER:HA	2.21	0.41
1:G:269:GLU:HA	5:G:789:NAG:C1	2.51	0.41
2:C:26:PHE:CE2	2:C:67:PHE:HB3	2.55	0.41
2:C:72:LYS:H	2:C:72:LYS:HG2	1.75	0.41
2:C:128:VAL:HG23	2:C:141:GLY:O	2.21	0.41
1:G:455:THR:HG23	1:G:455:THR:O	2.19	0.41
4:H:89:ASP:OD1	4:H:89:ASP:N	2.46	0.41
4:H:114:PHE:O	4:H:115:LEU:HD23	2.21	0.41
1:G:105:HIS:HB2	1:G:479:TRP:CD1	2.56	0.41
1:G:120:VAL:HG13	1:G:434:MET:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:CYS:HB2	2:C:28:TRP:HZ2	1.84	0.41
2:C:37:LEU:HD23	2:C:37:LEU:N	2.36	0.41
2:C:79:SER:OG	2:C:96:LEU:HA	2.21	0.41
2:C:138:ILE:O	2:C:138:ILE:HG13	2.21	0.41
3:L:15:PRO:HD3	3:L:108:ILE:HG22	2.02	0.41
1:G:333:LEU:HB3	1:G:414:ILE:HB	2.02	0.41
1:G:340:ASN:O	1:G:343:GLU:HB2	2.21	0.41
1:G:371:ILE:HD11	1:G:473:GLY:HA3	2.02	0.41
2:C:93:VAL:HG21	6:C:212:HOH:O	2.21	0.41
3:L:144:ARG:CG	3:L:165:VAL:HG11	2.51	0.41
1:G:279:ASN:HB3	1:G:282:LYS:HG2	2.03	0.40
2:C:74:LEU:HD12	2:C:74:LEU:HA	1.94	0.40
2:C:100:LEU:HB2	2:C:170:PHE:CD1	2.56	0.40
3:L:107:GLU:CG	3:L:108:ILE:N	2.84	0.40
4:H:185:LEU:HD13	4:H:191:TYR:CE1	2.56	0.40
1:G:432:LYS:HE3	1:G:432:LYS:HB2	1.97	0.40
3:L:6:GLN:OE1	3:L:101:GLY:HA3	2.21	0.40
4:H:40:ALA:O	4:H:43:GLN:HB2	2.22	0.40
1:G:414:ILE:HG22	1:G:416:LEU:HD13	2.03	0.40
4:H:141:PRO:CG	4:H:153:LEU:HD13	2.48	0.40
1:G:93:PHE:CE2	1:G:487:LYS:HG2	2.56	0.40
1:G:207:LYS:HD3	1:G:436:ALA:HB3	2.04	0.40
1:G:344:GLN:HG2	5:G:789:NAG:H83	2.03	0.40
3:L:79:GLN:HB2	3:L:82:ASP:CG	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	304/313 (97%)	251 (83%)	43 (14%)	10 (3%)	4 15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	179/185 (97%)	136 (76%)	38 (21%)	5 (3%)	5 19
3	L	212/214 (99%)	167 (79%)	32 (15%)	13 (6%)	1 4
4	H	227/229 (99%)	188 (83%)	32 (14%)	7 (3%)	4 16
All	All	922/941 (98%)	742 (80%)	145 (16%)	35 (4%)	3 13

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	220	PRO
1	G	268	GLU
1	G	475	MET
3	L	26	SER
3	L	76	SER
1	G	276	ASN
1	G	409	ASN
1	G	464	GLY
2	C	180	GLN
3	L	78	LEU
3	L	164	SER
3	L	184	SER
4	H	103	GLU
4	H	142	SER
1	G	253	PRO
1	G	267	GLU
1	G	407	LEU
2	C	105	ASP
2	C	154	SER
3	L	84	ALA
3	L	140	ASN
3	L	160	ASN
4	H	208	THR
4	H	53	THR
4	H	162	PRO
2	C	68	PRO
2	C	109	LEU
3	L	213	ARG
4	H	63	HIS
3	L	44	PRO
4	H	228	PRO
1	G	441	GLY
3	L	112	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	130	GLY
3	L	159	GLY

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	G	271/276 (98%)	256 (94%)	15 (6%)	21 53
2	C	164/167 (98%)	149 (91%)	15 (9%)	9 28
3	L	184/184 (100%)	169 (92%)	15 (8%)	11 32
4	H	193/193 (100%)	181 (94%)	12 (6%)	18 47
All	All	812/820 (99%)	755 (93%)	57 (7%)	15 41

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	103	GLN
1	G	123	THR
1	G	126	CYS
1	G	205	CYS
1	G	211	GLU
1	G	268	GLU
1	G	273	ARG
1	G	339	GLU
1	G	355	ASN
1	G	416	LEU
1	G	418	CYS
1	G	432	LYS
1	G	444	ARG
1	G	478	ASN
1	G	488	VAL
2	C	2	LYS
2	C	40	GLN
2	C	58	ARG
2	C	69	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	72	LYS
2	C	73	ASN
2	C	76	ILE
2	C	77	GLU
2	C	89	GLN
2	C	148	GLN
2	C	152	GLN
2	C	167	LYS
2	C	170	PHE
2	C	179	PHE
2	C	180	GLN
3	L	3	GLU
3	L	53	THR
3	L	74	THR
3	L	90	GLN
3	L	105	ARG
3	L	107	GLU
3	L	108	ILE
3	L	116	SER
3	L	139	ASN
3	L	145	GLU
3	L	156	LEU
3	L	162	GLN
3	L	169	LYS
3	L	171	LYS
3	L	181	LEU
4	H	1	GLN
4	H	2	VAL
4	H	38	ARG
4	H	53	THR
4	H	55	LEU
4	H	60	TYR
4	H	67	ARG
4	H	85	ASN
4	H	89	ASP
4	H	120	GLN
4	H	125	THR
4	H	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	92	ASN
1	G	114	GLN
1	G	246	GLN
1	G	340	ASN
1	G	355	ASN
1	G	362	ASN
1	G	478	ASN
2	C	32	ASN
2	C	33	GLN
2	C	73	ASN
2	C	103	ASN
2	C	110	GLN
2	C	165	GLN
3	L	149	GLN
4	H	1	GLN
4	H	3	GLN
4	H	85	ASN
4	H	120	GLN
4	H	207	GLN
4	H	214	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	G	963	1	14,14,15	0.68	0	17,19,21	0.73	0
5	NAG	G	795	1	14,14,15	0.55	0	17,19,21	0.67	0
5	NAG	G	762	1	14,14,15	0.64	0	17,19,21	0.73	1 (5%)
5	NAG	G	776	1	14,14,15	0.60	0	17,19,21	0.82	1 (5%)
5	NAG	G	734	1	14,14,15	0.62	0	17,19,21	0.55	0
5	NAG	G	948	1	14,14,15	0.78	0	17,19,21	0.67	1 (5%)
5	NAG	G	886	1	14,14,15	0.68	0	17,19,21	0.99	1 (5%)
5	NAG	G	856	1	14,14,15	0.67	0	17,19,21	0.65	0
5	NAG	G	588	1	14,14,15	0.56	0	17,19,21	0.69	0
5	NAG	G	789	1	14,14,15	0.63	0	17,19,21	0.72	1 (5%)
5	NAG	G	697	1	14,14,15	0.62	0	17,19,21	0.72	0
5	NAG	G	894	1	14,14,15	0.56	0	17,19,21	0.63	0
5	NAG	G	908	1	14,14,15	0.57	0	17,19,21	0.60	0
5	NAG	G	741	1	14,14,15	0.61	0	17,19,21	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	963	1	-	5/6/23/26	0/1/1/1
5	NAG	G	795	1	-	2/6/23/26	0/1/1/1
5	NAG	G	762	1	-	6/6/23/26	0/1/1/1
5	NAG	G	776	1	-	2/6/23/26	0/1/1/1
5	NAG	G	734	1	-	5/6/23/26	0/1/1/1
5	NAG	G	948	1	-	4/6/23/26	0/1/1/1
5	NAG	G	886	1	-	4/6/23/26	0/1/1/1
5	NAG	G	856	1	-	4/6/23/26	0/1/1/1
5	NAG	G	588	1	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	G	789	1	-	3/6/23/26	0/1/1/1
5	NAG	G	697	1	-	5/6/23/26	0/1/1/1
5	NAG	G	894	1	-	4/6/23/26	0/1/1/1
5	NAG	G	908	1	-	2/6/23/26	0/1/1/1
5	NAG	G	741	1	1/1/5/7	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	886	NAG	C2-N2-C7	-2.76	118.97	122.90
5	G	762	NAG	C2-N2-C7	-2.39	119.50	122.90
5	G	776	NAG	C2-N2-C7	-2.36	119.55	122.90
5	G	948	NAG	C2-N2-C7	-2.13	119.87	122.90
5	G	789	NAG	C2-N2-C7	-2.11	119.90	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	588	NAG	C1
5	G	741	NAG	C1

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	588	NAG	C8-C7-N2-C2
5	G	588	NAG	O7-C7-N2-C2
5	G	697	NAG	C8-C7-N2-C2
5	G	697	NAG	O7-C7-N2-C2
5	G	734	NAG	C8-C7-N2-C2
5	G	734	NAG	O7-C7-N2-C2
5	G	741	NAG	C8-C7-N2-C2
5	G	741	NAG	O7-C7-N2-C2
5	G	762	NAG	C1-C2-N2-C7
5	G	762	NAG	C8-C7-N2-C2
5	G	762	NAG	O7-C7-N2-C2
5	G	776	NAG	C8-C7-N2-C2
5	G	776	NAG	O7-C7-N2-C2
5	G	789	NAG	C8-C7-N2-C2
5	G	789	NAG	O7-C7-N2-C2
5	G	795	NAG	C8-C7-N2-C2
5	G	795	NAG	O7-C7-N2-C2
5	G	856	NAG	C8-C7-N2-C2
5	G	856	NAG	O7-C7-N2-C2
5	G	886	NAG	C8-C7-N2-C2
5	G	886	NAG	O7-C7-N2-C2
5	G	894	NAG	C8-C7-N2-C2
5	G	894	NAG	O7-C7-N2-C2
5	G	908	NAG	C8-C7-N2-C2
5	G	908	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	G	948	NAG	C8-C7-N2-C2
5	G	948	NAG	O7-C7-N2-C2
5	G	963	NAG	C8-C7-N2-C2
5	G	963	NAG	O7-C7-N2-C2
5	G	894	NAG	O5-C5-C6-O6
5	G	588	NAG	O5-C5-C6-O6
5	G	963	NAG	O5-C5-C6-O6
5	G	894	NAG	C4-C5-C6-O6
5	G	762	NAG	O5-C5-C6-O6
5	G	697	NAG	C1-C2-N2-C7
5	G	697	NAG	C4-C5-C6-O6
5	G	762	NAG	C4-C5-C6-O6
5	G	886	NAG	O5-C5-C6-O6
5	G	697	NAG	O5-C5-C6-O6
5	G	588	NAG	C4-C5-C6-O6
5	G	886	NAG	C4-C5-C6-O6
5	G	948	NAG	C4-C5-C6-O6
5	G	963	NAG	C4-C5-C6-O6
5	G	948	NAG	O5-C5-C6-O6
5	G	789	NAG	O5-C5-C6-O6
5	G	856	NAG	C4-C5-C6-O6
5	G	734	NAG	C4-C5-C6-O6
5	G	734	NAG	C3-C2-N2-C7
5	G	762	NAG	C3-C2-N2-C7
5	G	856	NAG	C3-C2-N2-C7
5	G	963	NAG	C3-C2-N2-C7
5	G	734	NAG	O5-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	963	NAG	1	0
5	G	762	NAG	1	0
5	G	776	NAG	1	0
5	G	734	NAG	1	0
5	G	948	NAG	1	0
5	G	856	NAG	2	0
5	G	789	NAG	4	0
5	G	697	NAG	1	0
5	G	894	NAG	2	0
5	G	908	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.