Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:51 AM GMT

PDB ID	:	3JWO
Title	:	Structure of HIV-1 gp120 with gp41-Interactive Region: Layered Architecture and Basis of Conformational Mobility
Authors	:	Pancera, M.; Majeed, S.; Huang, C.C.; Kwon, Y.D.; Zhou, T.; Robinson, J.E.; Sodroski, J.; Wyatt, R.; Kwong, P.D.
Deposited on	:	2009-09-18
Resolution	:	3.51 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:

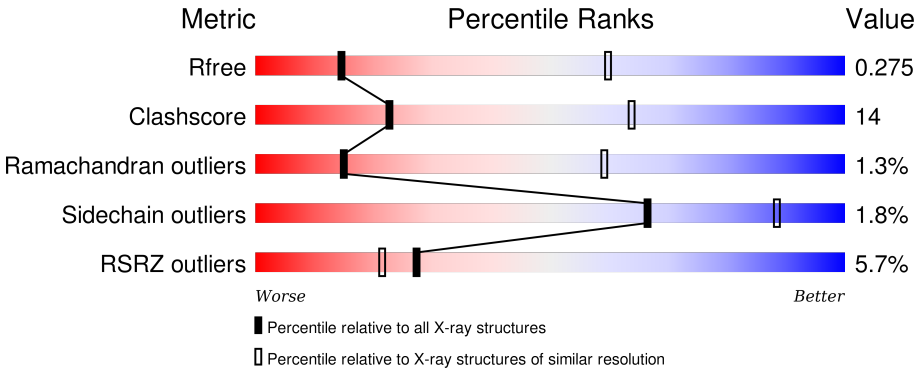
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 3.51 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	1089 (3.64-3.40)
Clashscore	102246	1197 (3.64-3.40)
Ramachandran outliers	100387	1159 (3.64-3.40)
Sidechain outliers	100360	1160 (3.64-3.40)
RSRZ outliers	91569	1096 (3.64-3.40)

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	357	67% 31%
2	C	184	71% 28%
3	L	209	9% 74% 25%
4	H	220	15% 75% 25%

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	A	730	-	-	-	X
5	NAG	A	734	X	-	-	-
5	NAG	A	897	-	-	-	X
5	NAG	A	948	X	-	-	X
6	NAG	A	789	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7597 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 HIV-1 GP120 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2747	1736	471	520	20			

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	184	Total	C	N	O	S	0	0	0
			1432	896	250	281	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1000	MET	-	INITIATING METHIONINE	UNP P01730

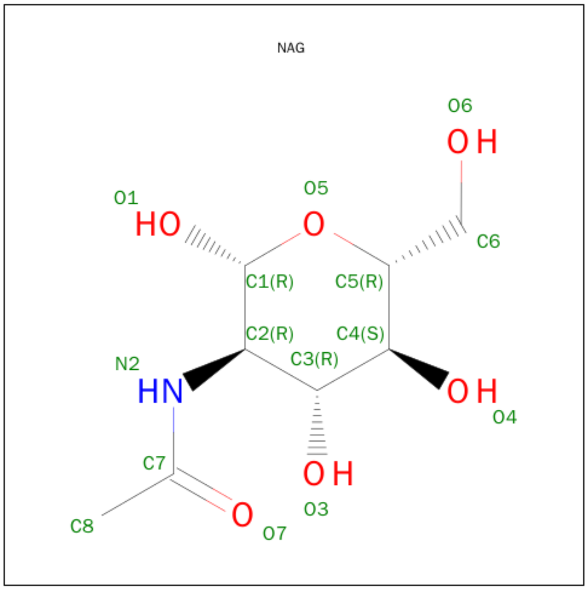
- Molecule 3 is a protein called FAB 48D LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	209	Total	C	N	O	S	0	0	0
			1600	1004	266	325	5			

- Molecule 4 is a protein called FAB 48D Heavy CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	220	Total	C	N	O	S	0	0	0
			1654	1048	267	332	7			

- Molecule 5 is SUGAR (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
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

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

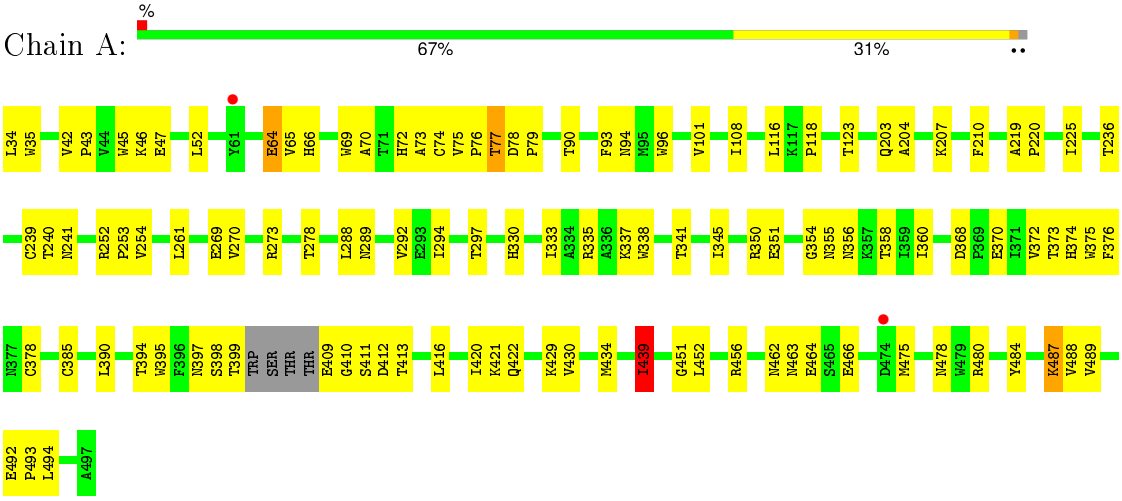
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total C N O 24 14 1 9	0	0

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.

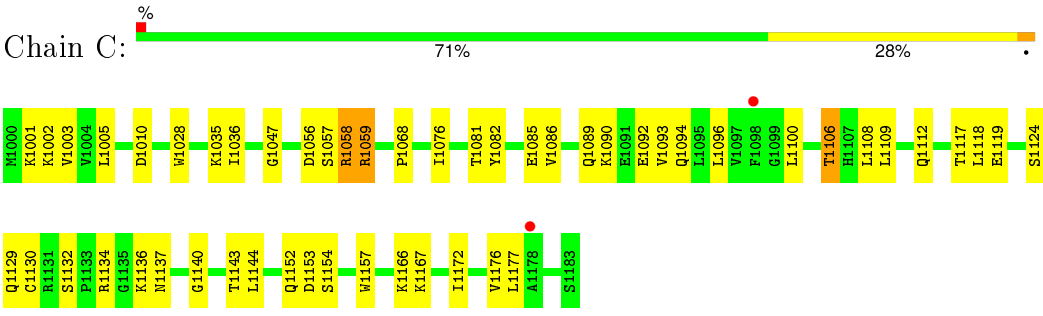
- Molecule 1: HIV-1 GP120 ENVELOPE GLYCOPROTEIN

Chain A:



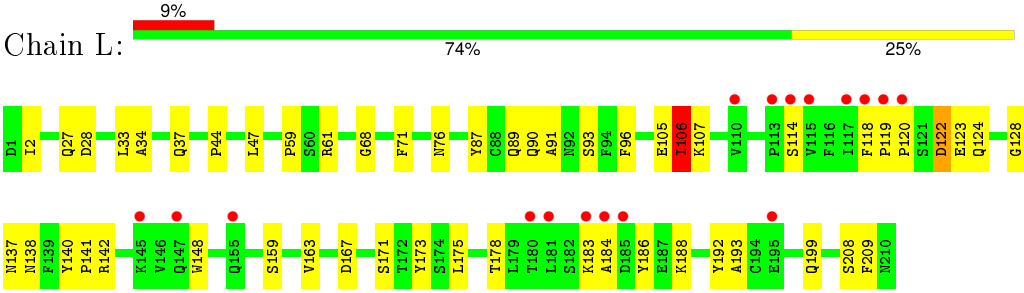
- Molecule 2: T-cell surface glycoprotein CD4

Chain C:



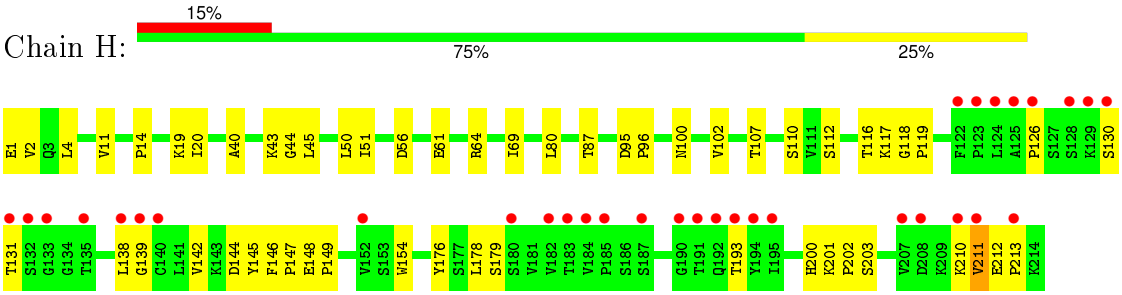
- Molecule 3: FAB 48D LIGHT CHAIN

Chain L:



- Molecule 4: FAB 48D Heavy CHAIN

Chain H:


15%
75%
25%
E1 V2 Q3 L4 V11 P14 K19 I20 A40 K43 G44 L45 L50 I51 D56 E61 R64 I69 L80 T87 D95 P96 N100 V102 T107 S110 V111 S112 T116 K117 G118 P119 F122 P123 L124 A125 P126 S127 S128 K129 S130
T131 S132 G133 G134 T135 L138 G139 C140 L141 V142 K143 D144 Y145 F146 P147 E148 P149 V152 S153 W154 Y176 S177 L178 S179 S180 V181 V182 T183 V184 P185 S186 S187 G190 T191 Q192 T193 Y194 I195 H200 K201 P202 S203 V207 D208 K209 K210 V211 E212 P213 K214

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	190.00Å 190.00Å 103.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.09 – 3.51 41.09 – 3.51	Depositor EDS
% Data completeness (in resolution range)	83.8 (41.09-3.51) 83.8 (41.09-3.51)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.257 , 0.273 0.255 , 0.275	Depositor DCC
R_{free} test set	2000 reflections (10.85%)	DCC
Wilson B-factor (Å^2)	84.4	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 79.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	2 of 21948 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7597	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: FUL, 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	A	0.26	0/2811	0.44	0/3827
2	C	0.27	0/1452	0.45	0/1955
3	L	0.25	0/1635	0.66	3/2221 (0.1%)
4	H	0.23	0/1695	0.42	0/2311
All	All	0.25	0/7593	0.49	3/10314 (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
3	L	0	1
6	A	1	0
All	All	1	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	106	ILE	CA-C-N	-14.96	84.30	117.20
3	L	106	ILE	O-C-N	14.29	145.57	122.70
3	L	106	ILE	C-N-CA	-12.89	89.47	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	789	NAG	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	106	ILE	Mainchain

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	2747	0	2664	96	0
2	C	1432	0	1460	39	0
3	L	1600	0	1552	33	0
4	H	1654	0	1613	40	0
5	A	140	0	130	3	0
6	A	24	0	22	0	0
All	All	7597	0	7441	204	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 14.

All (204) 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:398:SER:HA	1:A:399:THR:C	1.48	1.22
3:L:106:ILE:CG2	3:L:107:LYS:H	1.50	1.16
3:L:106:ILE:HG22	3:L:107:LYS:H	0.99	1.13
3:L:106:ILE:HG22	3:L:107:LYS:N	1.66	1.11
1:A:398:SER:CA	1:A:399:THR:C	2.33	0.95
4:H:126:PRO:HD3	4:H:138:LEU:HD13	1.54	0.90
1:A:492:GLU:HB3	1:A:493:PRO:HD2	1.54	0.88
1:A:335:ARG:NE	1:A:411:SER:HB3	1.90	0.86
1:A:34:LEU:O	1:A:35:TRP:HB2	1.75	0.86
1:A:335:ARG:CZ	1:A:411:SER:HB3	2.07	0.84
2:C:1085:GLU:HG2	2:C:1090:LYS:HG3	1.57	0.84
3:L:106:ILE:CG2	3:L:107:LYS:N	2.22	0.83
2:C:1058:ARG:HH12	2:C:1059:ARG:HH11	1.24	0.82
1:A:204:ALA:HB2	3:L:28:ASP:HB3	1.62	0.82
1:A:45:TRP:CD1	1:A:489:VAL:HG21	2.16	0.80
2:C:1058:ARG:NH1	2:C:1059:ARG:HH11	1.79	0.79
2:C:1166:LYS:HD3	2:C:1167:LYS:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLU:HA	1:A:355:ASN:OD1	1.88	0.74
1:A:398:SER:HA	1:A:399:THR:O	1.88	0.72
4:H:116:THR:HG22	4:H:203:SER:HB3	1.72	0.72
3:L:89:GLN:NE2	3:L:96:PHE:HB3	2.05	0.71
2:C:1106:THR:HB	2:C:1112:GLN:HG3	1.73	0.71
1:A:335:ARG:NH2	1:A:411:SER:HB3	2.05	0.71
4:H:20:ILE:HG21	4:H:107:THR:HG21	1.75	0.69
3:L:89:GLN:HE21	3:L:96:PHE:HB3	1.60	0.67
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.77	0.67
1:A:492:GLU:HB3	1:A:493:PRO:CD	2.25	0.66
1:A:412:ASP:O	1:A:413:THR:CG2	2.43	0.66
4:H:200:HIS:CE1	4:H:202:PRO:HB2	2.30	0.66
1:A:207:LYS:HB3	1:A:439:ILE:HD11	1.76	0.66
4:H:116:THR:HA	4:H:146:PHE:O	1.94	0.66
1:A:398:SER:CA	1:A:399:THR:O	2.43	0.66
2:C:1058:ARG:HH12	2:C:1059:ARG:NH1	1.94	0.65
1:A:77:THR:HG22	1:A:78:ASP:H	1.61	0.65
1:A:64:GLU:OE2	1:A:66:HIS:HB2	1.96	0.65
2:C:1100:LEU:HD21	2:C:1172:ILE:HD11	1.79	0.65
1:A:420:ILE:H	1:A:420:ILE:HD12	1.64	0.63
1:A:360:ILE:HG12	1:A:394:THR:HG23	1.81	0.62
1:A:43:PRO:HA	1:A:494:LEU:HD23	1.82	0.62
3:L:193:ALA:HB2	3:L:208:SER:HB3	1.82	0.62
1:A:78:ASP:HB2	1:A:79:PRO:HA	1.82	0.61
2:C:1134:ARG:HD3	2:C:1152:GLN:HB3	1.82	0.61
4:H:61:GLU:HA	4:H:64:ARG:NH1	2.15	0.61
4:H:138:LEU:HD11	4:H:211:VAL:HG11	1.82	0.61
2:C:1132:SER:HB3	2:C:1136:LYS:HB3	1.83	0.60
2:C:1086:VAL:O	2:C:1089:GLN:HG2	2.01	0.60
4:H:87:THR:HG23	4:H:110:SER:HA	1.82	0.60
4:H:119:PRO:HB3	4:H:142:VAL:CG1	2.32	0.60
1:A:45:TRP:HD1	1:A:489:VAL:HG21	1.66	0.59
1:A:207:LYS:CB	1:A:439:ILE:HD11	2.32	0.59
1:A:430:VAL:HG11	2:C:1059:ARG:HB2	1.83	0.58
2:C:1140:GLY:HA3	2:C:1144:LEU:HG	1.85	0.58
2:C:1057:SER:HB2	2:C:1068:PRO:O	2.03	0.58
1:A:335:ARG:HE	1:A:411:SER:HB3	1.63	0.58
1:A:412:ASP:C	1:A:413:THR:HG23	2.24	0.58
1:A:108:ILE:HD12	1:A:253:PRO:HB3	1.83	0.58
2:C:1134:ARG:HH21	2:C:1136:LYS:HE2	1.69	0.57
1:A:269:GLU:HA	1:A:289:ASN:HD22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:NH2	1:A:411:SER:CB	2.68	0.57
2:C:1003:VAL:HG22	2:C:1094:GLN:HB3	1.86	0.56
1:A:207:LYS:HG3	1:A:439:ILE:CG1	2.36	0.56
1:A:207:LYS:CG	1:A:439:ILE:HD11	2.36	0.55
1:A:78:ASP:HB2	1:A:79:PRO:CA	2.37	0.55
4:H:1:GLU:HG3	4:H:2:VAL:H	1.70	0.55
3:L:128:GLY:HA2	3:L:183:LYS:HD2	1.88	0.55
1:A:335:ARG:HH21	1:A:411:SER:CB	2.20	0.55
3:L:33:LEU:HD22	3:L:71:PHE:CG	2.42	0.54
1:A:412:ASP:O	1:A:413:THR:HG22	2.07	0.54
1:A:451:GLY:C	1:A:452:LEU:HD12	2.29	0.53
1:A:398:SER:HB2	1:A:399:THR:O	2.09	0.53
4:H:138:LEU:HD11	4:H:211:VAL:CG1	2.39	0.53
1:A:412:ASP:O	1:A:413:THR:HG23	2.08	0.53
1:A:207:LYS:HG3	1:A:439:ILE:HG12	1.91	0.52
2:C:1130:CYS:SG	2:C:1144:LEU:HD22	2.50	0.52
2:C:1118:LEU:HD22	2:C:1128:VAL:HG22	1.90	0.52
2:C:1154:SER:HB2	2:C:1176:VAL:HG12	1.90	0.52
1:A:398:SER:CB	1:A:399:THR:O	2.58	0.52
4:H:4:LEU:HD11	4:H:102:VAL:HG23	1.91	0.52
3:L:192:TYR:HB2	3:L:209:PHE:CE2	2.44	0.52
3:L:59:PRO:HB3	3:L:61:ARG:NH1	2.25	0.51
1:A:207:LYS:HG3	1:A:439:ILE:HD11	1.93	0.51
4:H:193:THR:HG23	4:H:210:LYS:HE3	1.93	0.51
4:H:117:LYS:HD3	4:H:118:GLY:N	2.26	0.50
3:L:91:ALA:HB1	4:H:100:ASN:O	2.11	0.50
4:H:148:GLU:HB3	4:H:149:PRO:HA	1.94	0.50
1:A:420:ILE:HD12	1:A:420:ILE:N	2.26	0.50
1:A:46:LYS:HE2	1:A:492:GLU:OE2	2.11	0.50
1:A:90:THR:OG1	1:A:240:THR:HG22	2.12	0.50
1:A:341:THR:O	1:A:345:ILE:HG13	2.12	0.50
2:C:1089:GLN:C	2:C:1090:LYS:HD2	2.32	0.50
3:L:167:ASP:O	3:L:171:SER:HA	2.12	0.49
1:A:350:ARG:HG2	1:A:355:ASN:HA	1.94	0.49
1:A:294:ILE:HD12	1:A:333:ILE:HD11	1.95	0.49
4:H:200:HIS:HE1	4:H:202:PRO:HB2	1.78	0.49
1:A:412:ASP:C	1:A:413:THR:CG2	2.81	0.49
3:L:184:ALA:O	3:L:188:LYS:HD3	2.12	0.49
2:C:1153:ASP:HB3	2:C:1157:TRP:HZ2	1.77	0.49
3:L:90:GLN:O	3:L:96:PHE:HA	2.12	0.49
4:H:145:TYR:HD1	4:H:200:HIS:HE2	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:730:NAG:HN2	5:A:730:NAG:H5	1.77	0.48
2:C:1132:SER:CB	2:C:1136:LYS:HB3	2.43	0.48
1:A:47:GLU:HG2	1:A:487:LYS:HE3	1.94	0.48
4:H:119:PRO:CB	4:H:142:VAL:HG13	2.43	0.48
1:A:70:ALA:O	1:A:74:CYS:HB2	2.13	0.48
1:A:75:VAL:HG13	1:A:76:PRO:HD2	1.96	0.47
3:L:33:LEU:HG	3:L:34:ALA:N	2.29	0.47
1:A:338:TRP:CE2	1:A:390:LEU:HD22	2.49	0.47
2:C:1082:TYR:O	2:C:1093:VAL:HG12	2.15	0.47
1:A:42:VAL:HG13	1:A:43:PRO:HD2	1.97	0.47
1:A:219:ALA:HB2	1:A:225:ILE:HG13	1.97	0.47
1:A:94:ASN:HA	1:A:236:THR:HG22	1.97	0.46
1:A:373:THR:HB	1:A:385:CYS:O	2.15	0.46
2:C:1076:ILE:HG13	2:C:1119:GLU:CD	2.35	0.46
1:A:270:VAL:HG22	1:A:288:LEU:HA	1.98	0.46
3:L:140:TYR:CG	3:L:141:PRO:HA	2.51	0.46
2:C:1166:LYS:CD	2:C:1167:LYS:H	2.24	0.46
4:H:148:GLU:OE1	4:H:149:PRO:HA	2.16	0.46
4:H:51:ILE:HA	4:H:56:ASP:O	2.15	0.46
1:A:72:HIS:CG	1:A:72:HIS:O	2.69	0.46
1:A:108:ILE:CD1	1:A:253:PRO:HB3	2.46	0.46
1:A:52:LEU:N	1:A:52:LEU:HD12	2.31	0.46
1:A:77:THR:HG22	1:A:78:ASP:N	2.27	0.45
4:H:14:PRO:HD3	4:H:112:SER:O	2.15	0.45
2:C:1058:ARG:HD3	2:C:1058:ARG:HA	1.49	0.45
4:H:11:VAL:HG22	4:H:147:PRO:HG2	1.98	0.45
1:A:420:ILE:HG22	1:A:421:LYS:N	2.32	0.45
4:H:69:ILE:HG12	4:H:80:LEU:HD13	1.98	0.45
2:C:1154:SER:HB2	2:C:1176:VAL:CG1	2.47	0.44
2:C:1124:SER:O	2:C:1126:PRO:HD3	2.17	0.44
1:A:219:ALA:HA	1:A:220:PRO:HD3	1.79	0.44
1:A:96:TRP:HD1	1:A:236:THR:HG21	1.82	0.44
3:L:124:GLN:HG2	3:L:129:THR:O	2.18	0.44
1:A:335:ARG:HE	1:A:411:SER:CB	2.30	0.44
3:L:159:SER:HA	3:L:178:THR:O	2.16	0.44
1:A:422:GLN:O	1:A:434:MET:HA	2.17	0.44
1:A:292:VAL:HG13	1:A:337:LYS:HE3	1.99	0.44
2:C:1129:GLN:NE2	2:C:1137:ASN:HB3	2.32	0.44
1:A:358:THR:HG23	1:A:395:TRP:O	2.18	0.44
1:A:118:PRO:HD2	1:A:203:GLN:NE2	2.32	0.44
1:A:409:GLU:HG2	1:A:409:GLU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:145:TYR:CZ	4:H:176:TYR:HB2	2.53	0.43
3:L:128:GLY:CA	3:L:183:LYS:HD2	2.47	0.43
3:L:122:ASP:OD2	3:L:123:GLU:HG3	2.18	0.43
1:A:207:LYS:HG3	1:A:439:ILE:CD1	2.48	0.43
1:A:101:VAL:HG21	1:A:480:ARG:HG2	2.00	0.43
2:C:1117:THR:HG23	2:C:1143:THR:HG22	2.00	0.43
1:A:294:ILE:HG23	1:A:294:ILE:O	2.19	0.43
4:H:119:PRO:HB3	4:H:142:VAL:HG12	2.01	0.43
4:H:119:PRO:HB3	4:H:142:VAL:HG13	2.01	0.43
2:C:1005:LEU:CD2	2:C:1096:LEU:HB2	2.48	0.43
3:L:163:VAL:HG22	3:L:175:LEU:HD12	2.00	0.43
1:A:65:VAL:HG21	1:A:210:PHE:CD1	2.53	0.43
4:H:95:ASP:N	4:H:96:PRO:HD3	2.33	0.42
3:L:87:TYR:OH	4:H:44:GLY:HA2	2.19	0.42
4:H:50:LEU:C	4:H:50:LEU:HD12	2.40	0.42
1:A:34:LEU:N	1:A:34:LEU:HD22	2.34	0.42
2:C:1118:LEU:HD22	2:C:1128:VAL:CG2	2.48	0.42
2:C:1035:LYS:O	2:C:1047:GLY:HA3	2.20	0.42
1:A:456:ARG:HD2	1:A:466:GLU:OE1	2.20	0.42
1:A:475:MET:HA	1:A:478:ASN:OD1	2.19	0.42
5:A:730:NAG:H62	5:A:734:NAG:O7	2.20	0.42
1:A:394:THR:HG22	1:A:397:ASN:HB2	2.01	0.42
1:A:123:THR:HG21	1:A:429:LYS:HE3	2.02	0.42
2:C:1134:ARG:NH1	2:C:1152:GLN:HB2	2.35	0.42
1:A:368:ASP:O	1:A:372:VAL:HG23	2.19	0.42
1:A:330:HIS:HA	1:A:416:LEU:O	2.20	0.42
1:A:252:ARG:HA	1:A:253:PRO:HD3	1.76	0.42
3:L:120:PRO:HG2	3:L:186:TYR:CZ	2.55	0.42
1:A:350:ARG:NH2	1:A:356:ASN:HA	2.35	0.41
4:H:146:PHE:HA	4:H:147:PRO:HA	1.77	0.41
4:H:212:GLU:HA	4:H:213:PRO:HD3	1.75	0.41
1:A:69:TRP:O	1:A:73:ALA:HB3	2.20	0.41
1:A:370:GLU:HA	1:A:375:TRP:HB2	2.01	0.41
3:L:118:PHE:HA	3:L:119:PRO:HD3	1.87	0.41
1:A:480:ARG:O	1:A:484:TYR:HB3	2.20	0.41
2:C:1001:LYS:HG2	2:C:1002:LYS:N	2.35	0.41
3:L:44:PRO:CG	4:H:45:LEU:HD11	2.49	0.41
2:C:1108:LEU:O	2:C:1109:LEU:HB2	2.20	0.41
1:A:254:VAL:HG11	1:A:261:LEU:HB2	2.02	0.41
3:L:114:SER:HB2	3:L:137:ASN:HB3	2.03	0.41
1:A:273:ARG:NH2	1:A:484:TYR:CE2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:28:ASP:OD1	3:L:68:GLY:HA2	2.20	0.41
1:A:463:ASN:O	1:A:464:GLU:HB2	2.20	0.41
3:L:134:CYS:HB2	3:L:148:TRP:CZ2	2.55	0.41
4:H:201:LYS:N	4:H:202:PRO:CD	2.83	0.41
2:C:1028:TRP:O	2:C:1036:ILE:HB	2.21	0.41
4:H:178:LEU:HD12	4:H:179:SER:N	2.36	0.41
4:H:116:THR:CG2	4:H:203:SER:HB3	2.46	0.41
4:H:19:LYS:HA	4:H:80:LEU:O	2.21	0.41
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.89	0.41
1:A:376:PHE:HE2	1:A:378:CYS:HB2	1.84	0.41
2:C:1081:THR:CG2	2:C:1092:GLU:HG2	2.51	0.41
1:A:278:THR:HG22	5:A:776:NAG:H62	2.03	0.41
2:C:1144:LEU:HD12	2:C:1144:LEU:N	2.36	0.41
1:A:96:TRP:CD1	1:A:236:THR:HG21	2.56	0.41
1:A:368:ASP:OD2	2:C:1059:ARG:NH2	2.40	0.40
1:A:207:LYS:HA	1:A:207:LYS:HD3	1.93	0.40
4:H:118:GLY:HA2	4:H:119:PRO:HD3	1.91	0.40
4:H:139:GLY:HA2	4:H:154:TRP:CH2	2.55	0.40
1:A:409:GLU:HA	1:A:410:GLY:HA3	1.62	0.40
3:L:2:ILE:HD12	3:L:27:GLN:HB2	2.03	0.40
1:A:93:PHE:HE2	1:A:239:CYS:HB3	1.85	0.40
3:L:142:ARG:HB2	3:L:173:TYR:CE1	2.57	0.40
4:H:40:ALA:HB3	4:H:43:LYS:HB2	2.04	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	A	349/357 (98%)	300 (86%)	44 (13%)	5 (1%)	14 57
2	C	182/184 (99%)	168 (92%)	13 (7%)	1 (0%)	34 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	L	207/209 (99%)	190 (92%)	14 (7%)	3 (1%)	14 57
4	H	218/220 (99%)	193 (88%)	22 (10%)	3 (1%)	14 57
All	All	956/970 (99%)	851 (89%)	93 (10%)	12 (1%)	15 59

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	76	ASN
3	L	138	ASN
4	H	130	SER
4	H	144	ASP
1	A	241	ASN
1	A	354	GLY
2	C	1056	ASP
3	L	93	SER
4	H	131	THR
1	A	439	ILE
1	A	462	ASN
1	A	487	LYS

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	309/313 (99%)	303 (98%)	6 (2%)	65 87
2	C	166/166 (100%)	161 (97%)	5 (3%)	48 81
3	L	182/182 (100%)	179 (98%)	3 (2%)	70 90
4	H	185/185 (100%)	184 (100%)	1 (0%)	92 97
All	All	842/846 (100%)	827 (98%)	15 (2%)	66 88

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	GLU
1	A	77	THR
1	A	297	THR
1	A	374	HIS
1	A	439	ILE
1	A	488	VAL
2	C	1010	ASP
2	C	1058	ARG
2	C	1059	ARG
2	C	1106	THR
2	C	1177	LEU
3	L	105	GLU
3	L	122	ASP
3	L	199	GLN
4	H	211	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

2 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	789	1,6	14,14,15	0.52	0	15,19,21	1.01	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	FUL	A	790	6	10,10,11	0.56	0	14,14,16	0.76	1 (7%)

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
6	NAG	A	789	1,6	1/1/5/7	2/6/23/26	0/1/1/1
6	FUL	A	790	6	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	790	FUL	O5-C5-C6	2.06	109.53	106.13
6	A	789	NAG	O5-C5-C6	2.50	112.77	107.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	789	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	789	NAG	C8-C7-N2-C2
6	A	789	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

10 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	A	588	1	14,14,15	0.52	0	15,19,21	1.36	1 (6%)
5	NAG	A	730	1	14,14,15	0.46	0	15,19,21	0.86	1 (6%)
5	NAG	A	734	1	14,14,15	0.48	0	15,19,21	0.77	0
5	NAG	A	741	1	14,14,15	0.50	0	15,19,21	0.88	1 (6%)
5	NAG	A	762	1	14,14,15	0.48	0	15,19,21	0.95	1 (6%)
5	NAG	A	776	1	14,14,15	0.48	0	15,19,21	0.78	1 (6%)
5	NAG	A	886	1	14,14,15	0.48	0	15,19,21	0.73	0
5	NAG	A	892	1	14,14,15	0.51	0	15,19,21	1.02	1 (6%)
5	NAG	A	897	1	14,14,15	0.50	0	15,19,21	0.77	0
5	NAG	A	948	1	14,14,15	0.50	0	15,19,21	1.05	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	588	1	-	0/6/23/26	0/1/1/1
5	NAG	A	730	1	-	0/6/23/26	0/1/1/1
5	NAG	A	734	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	A	741	1	-	0/6/23/26	0/1/1/1
5	NAG	A	762	1	-	0/6/23/26	0/1/1/1
5	NAG	A	776	1	-	0/6/23/26	0/1/1/1
5	NAG	A	886	1	-	0/6/23/26	0/1/1/1
5	NAG	A	892	1	-	0/6/23/26	0/1/1/1
5	NAG	A	897	1	-	0/6/23/26	0/1/1/1
5	NAG	A	948	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	762	NAG	C1-O5-C5	2.05	114.85	112.25
5	A	741	NAG	C1-O5-C5	2.10	114.92	112.25
5	A	776	NAG	C1-O5-C5	2.10	114.92	112.25
5	A	730	NAG	C1-O5-C5	2.18	115.01	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	948	NAG	C1-O5-C5	2.74	115.73	112.25
5	A	892	NAG	C1-O5-C5	2.85	115.86	112.25
5	A	588	NAG	C1-O5-C5	4.50	117.96	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	948	NAG	C1
5	A	734	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	734	NAG	O7-C7-N2-C2
5	A	734	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	730	NAG	2	0
5	A	734	NAG	1	0
5	A	776	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

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	353/357 (98%)	0.03	2 (0%) 90 85	68, 98, 161, 262	0
2	C	184/184 (100%)	0.26	2 (1%) 82 74	86, 121, 182, 234	0
3	L	209/209 (100%)	0.65	18 (8%) 13 12	105, 173, 260, 460	0
4	H	220/220 (100%)	0.76	33 (15%) 3 3	95, 164, 306, 365	0
All	All	966/970 (99%)	0.38	55 (5%) 27 21	68, 124, 257, 460	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	183	THR	8.5
4	H	131	THR	7.3
4	H	194	TYR	7.2
4	H	138	LEU	6.3
4	H	139	GLY	6.2
4	H	132	SER	6.0
4	H	182	VAL	5.1
3	L	119	PRO	5.0
4	H	126	PRO	4.6
4	H	130	SER	4.4
3	L	184	ALA	4.0
4	H	211	VAL	3.9
3	L	114	SER	3.8
4	H	213	PRO	3.8
3	L	120	PRO	3.6
3	L	147	GLN	3.5
4	H	184	VAL	3.4
4	H	193	THR	3.1
4	H	192	GLN	3.1
3	L	185	ASP	3.0
4	H	128	SER	3.0

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Mol	Chain	Res	Type	RSRZ
4	H	210	LYS	3.0
4	H	125	ALA	2.9
4	H	180	SER	2.9
4	H	133	GLY	2.8
4	H	140	CYS	2.8
4	H	207	VAL	2.8
3	L	155	GLN	2.7
2	C	1098	PHE	2.6
3	L	195	GLU	2.6
3	L	115	VAL	2.6
4	H	195	ILE	2.6
4	H	187	SER	2.5
3	L	117	ILE	2.5
1	A	61	TYR	2.4
3	L	145	LYS	2.3
4	H	191	THR	2.3
3	L	180	THR	2.3
4	H	123	PRO	2.3
4	H	135	THR	2.3
2	C	1178	ALA	2.3
4	H	122	PHE	2.2
3	L	181	LEU	2.2
3	L	183	LYS	2.2
3	L	118	PHE	2.2
4	H	190	GLY	2.2
1	A	474	ASP	2.2
3	L	113	PRO	2.2
4	H	124	LEU	2.1
4	H	185	PRO	2.1
4	H	152	VAL	2.1
4	H	129	LYS	2.1
4	H	208	ASP	2.1
3	L	136	LEU	2.0
3	L	110	VAL	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)

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
6	NAG	A	789	14/15	0.90	0.18	-2.10	84,111,141,166	0
6	FUL	A	790	10/11	0.51	0.40	-	197,211,231,236	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	A	730	14/15	0.73	0.53	23.81	232,249,275,286	0
5	NAG	A	897	14/15	0.65	0.53	3.05	139,208,226,240	0
5	NAG	A	948	14/15	0.77	0.32	2.94	134,155,186,195	0
5	NAG	A	886	14/15	0.85	0.32	1.35	75,115,154,164	0
5	NAG	A	734	14/15	0.86	0.23	-0.05	145,167,194,207	0
5	NAG	A	776	14/15	0.84	0.24	-0.11	112,131,168,180	0
5	NAG	A	762	14/15	0.93	0.23	-0.23	75,80,100,100	0
5	NAG	A	892	14/15	0.82	0.29	-	102,144,192,206	0
5	NAG	A	741	14/15	0.67	0.43	-	215,224,236,239	0
5	NAG	A	588	14/15	0.80	0.26	-	95,145,161,167	0

6.5 Other polymers (i)

There are no such residues in this entry.