



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:28 AM BST

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

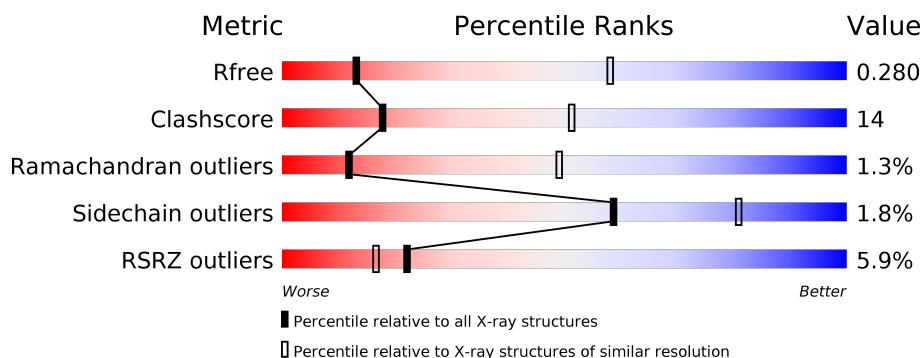
1 Overall quality at a glance

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}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	357	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> 67% 31% </div> </div>
2	C	184	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> 71% 28% </div> </div>
3	L	209	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> 74% 25% </div> </div>
4	H	220	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> 75% 25% </div> </div>
5	B	2	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> 50% 50% </div> </div>

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	B	1	X	-	-	-
6	NAG	A	730	-	-	-	X
6	NAG	A	734	X	-	-	-
6	NAG	A	741	-	-	-	X
6	NAG	A	897	-	-	-	X
6	NAG	A	948	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.

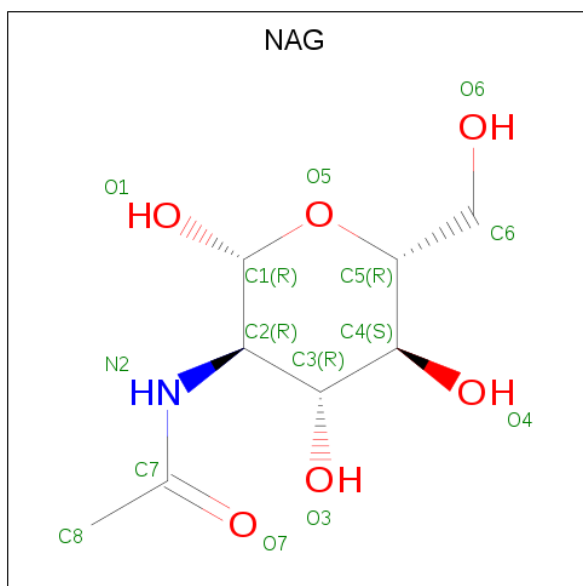
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	220	Total	C	N	O	S	0	0	0
			1654	1048	267	332	7			

- Molecule 5 is an oligosaccharide called beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	B	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

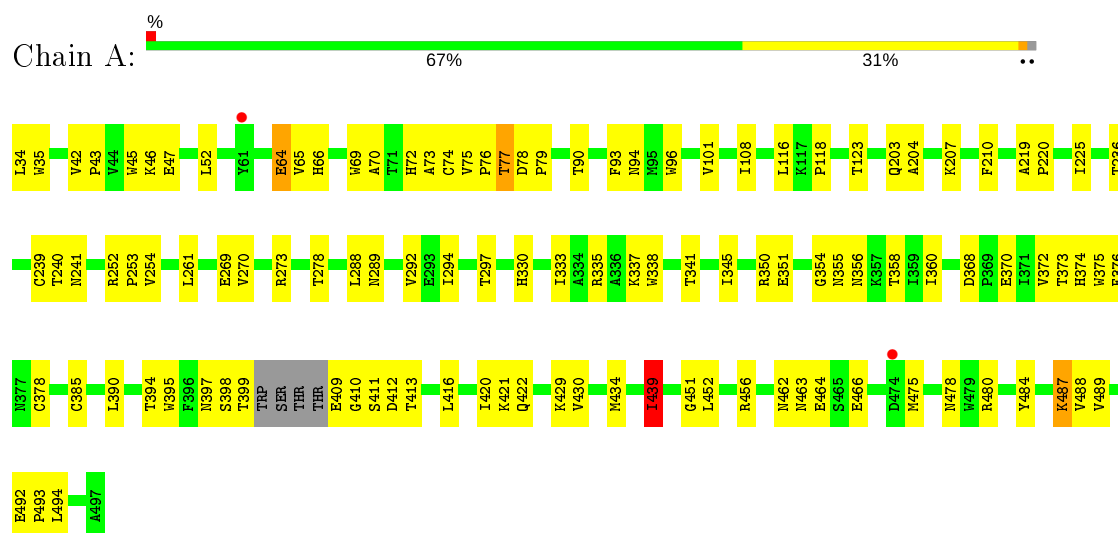


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1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

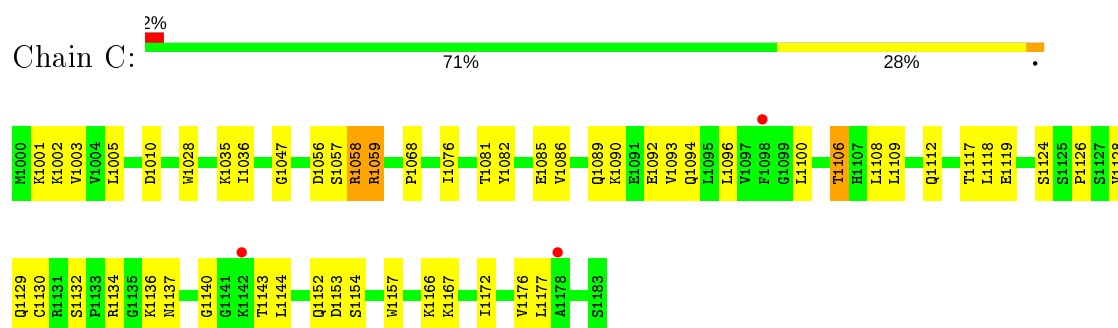
3 Residue-property plots [i](#)

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 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.

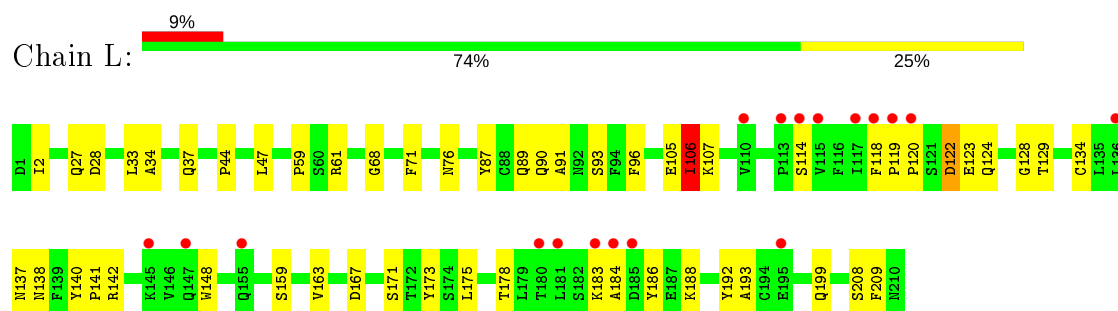
• Molecule 1: HIV-1 GP120 ENVELOPE GLYCOPROTEIN



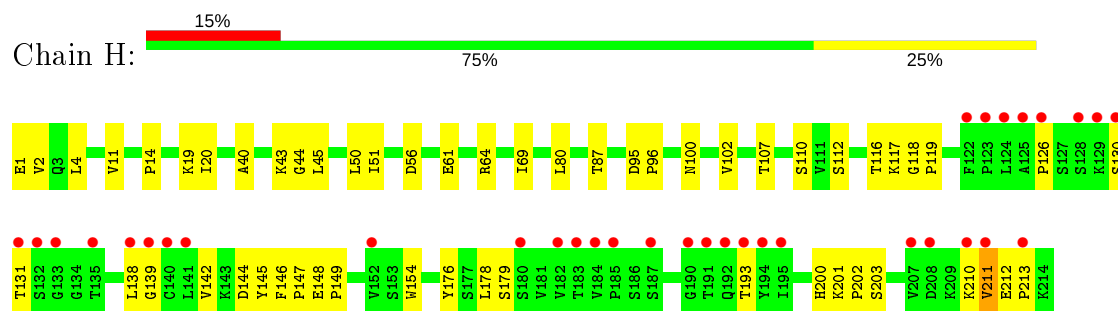
• Molecule 2: T-cell surface glycoprotein CD4



• Molecule 3: FAB 48D LIGHT CHAIN



● Molecule 4: FAB 48D Heavy CHAIN



● Molecule 5: beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	190.00 Å 190.00 Å 103.30 Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.48 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.257 , 0.273 0.258 , 0.280	Depositor DCC
R_{free} test set	2000 reflections (9.11%)	wwPDB-VP
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
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	106	ILE	Mainchain

5.2 Too-close contacts ⓘ

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	B	24	0	22	0	0
6	A	140	0	130	3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:77:THR:HG22	1:A:78:ASP:H	1.61	0.65
2:C:1058:ARG:HH12	2:C:1059:ARG:NH1	1.94	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:119:PRO:HB3	4:H:142:VAL:CG1	2.32	0.60
4:H:87:THR:HG23	4:H:110:SER:HA	1.82	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:1057:SER:HB2	2:C:1068:PRO:O	2.03	0.58
2:C:1140:GLY:HA3	2:C:1144:LEU:HG	1.85	0.58
1:A:335:ARG:HE	1:A:411:SER:HB3	1.63	0.58
1:A:108:ILE:HD12	1:A:253:PRO:HB3	1.83	0.58
1:A:412:ASP:C	1:A:413:THR:HG23	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:412:ASP:O	1:A:413:THR:HG23	2.08	0.53
4:H:138:LEU:HD11	4:H:211:VAL:CG1	2.39	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:341:THR:O	1:A:345:ILE:HG13	2.12	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
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:294:ILE:HD12	1:A:333:ILE:HD11	1.95	0.49
1:A:350:ARG:HG2	1:A:355:ASN:HA	1.94	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
2:C:1153:ASP:HB3	2:C:1157:TRP:HZ2	1.77	0.49
3:L:184:ALA:O	3:L:188:LYS:HD3	2.12	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
6:A:730:NAG:HN2	6: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:338:TRP:CE2	1:A:390:LEU:HD22	2.49	0.47
3:L:33:LEU:HG	3:L:34:ALA:N	2.29	0.47
2:C:1082:TYR:O	2:C:1093:VAL:HG12	2.15	0.47
1:A:219:ALA:HB2	1:A:225:ILE:HG13	1.97	0.47
1:A:42:VAL:HG13	1:A:43:PRO:HD2	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
1:A:270:VAL:HG22	1:A:288:LEU:HA	1.98	0.46
2:C:1076:ILE:HG13	2:C:1119:GLU:CD	2.35	0.46
3:L:140:TYR:CG	3:L:141:PRO:HA	2.51	0.46
1:A:72:HIS:CG	1:A:72:HIS:O	2.69	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: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
1:A:420:ILE:HG22	1:A:421:LYS:N	2.32	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
4:H:69:ILE:HG12	4:H:80:LEU:HD13	1.98	0.45
2:C:1124:SER:O	2:C:1126:PRO:HD3	2.17	0.44
2:C:1154:SER:HB2	2:C:1176:VAL:CG1	2.47	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
1:A:292:VAL:HG13	1:A:337:LYS:HE3	1.99	0.44
1:A:422:GLN:O	1:A:434:MET:HA	2.17	0.44
3:L:159:SER:HA	3:L:178:THR:O	2.16	0.44
1:A:358:THR:HG23	1:A:395:TRP:O	2.18	0.44
2:C:1129:GLN:NE2	2:C:1137:ASN:HB3	2.32	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
4:H:145:TYR:CZ	4:H:176:TYR:HB2	2.53	0.43
3:L:122:ASP:OD2	3:L:123:GLU:HG3	2.18	0.43
3:L:128:GLY:CA	3:L:183:LYS:HD2	2.47	0.43
1:A:207:LYS:HG3	1:A:439:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:1005:LEU:CD2	2:C:1096:LEU:HB2	2.48	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
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
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
2:C:1035:LYS:O	2:C:1047:GLY:HA3	2.20	0.42
6:A:730:NAG:H62	6:A:734:NAG:O7	2.20	0.42
1:A:123:THR:HG21	1:A:429:LYS:HE3	2.02	0.42
1:A:394:THR:HG22	1:A:397:ASN:HB2	2.01	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
1:A:370:GLU:HA	1:A:375:TRP:HB2	2.01	0.41
1:A:69:TRP:O	1:A:73:ALA:HB3	2.20	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
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
1:A:254:VAL:HG11	1:A:261:LEU:HB2	2.02	0.41
2:C:1108:LEU:O	2:C:1109:LEU:HB2	2.20	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
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
3:L:28:ASP:OD1	3:L:68:GLY:HA2	2.20	0.41
2:C:1028:TRP:O	2:C:1036:ILE:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:178:LEU:HD12	4:H:179:SER:N	2.36	0.41
4:H:201:LYS:N	4:H:202:PRO:CD	2.83	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	6:A:776:NAG:H62	2.03	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:96:TRP:CD1	1:A:236:THR:HG21	2.56	0.41
2:C:1144:LEU:HD12	2:C:1144:LEU:N	2.36	0.41
1:A:207:LYS:HA	1:A:207:LYS:HD3	1.93	0.40
1:A:368:ASP:OD2	2:C:1059:ARG:NH2	2.40	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
4:H:40:ALA:HB3	4:H:43:LYS:HB2	2.04	0.40
3:L:142:ARG:HB2	3:L:173:TYR:CE1	2.57	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%)	11	47
2	C	182/184 (99%)	168 (92%)	13 (7%)	1 (0%)	29	67
3	L	207/209 (99%)	190 (92%)	14 (7%)	3 (1%)	11	47
4	H	218/220 (99%)	193 (88%)	22 (10%)	3 (1%)	11	47
All	All	956/970 (99%)	851 (89%)	93 (10%)	12 (1%)	12	49

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 ⓘ

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%)	57	80
2	C	166/166 (100%)	161 (97%)	5 (3%)	41	71
3	L	182/182 (100%)	179 (98%)	3 (2%)	62	83
4	H	185/185 (100%)	184 (100%)	1 (0%)	88	95
All	All	842/846 (100%)	827 (98%)	15 (2%)	59	81

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

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Mol	Chain	Res	Type
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 monosaccharides 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	B	1	1,5	14,14,15	0.54	0	17,19,21	1.53	2 (11%)
5	FUL	B	2	5	10,10,11	0.65	0	14,14,16	0.54	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	B	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	FUL	B	2	5	-	-	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(°)	Ideal(°)
5	B	1	NAG	O5-C1-C2	4.02	117.64	111.29
5	B	1	NAG	O5-C5-C6	3.55	112.77	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1	NAG	C8-C7-N2-C2
5	B	1	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
6	NAG	A	892	1	14,14,15	0.53	0	17,19,21	1.11	2 (11%)
6	NAG	A	948	1	14,14,15	0.53	0	17,19,21	1.03	1 (5%)
6	NAG	A	897	1	14,14,15	0.53	0	17,19,21	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	730	1	14,14,15	0.49	0	17,19,21	0.84	1 (5%)
6	NAG	A	588	1	14,14,15	0.53	0	17,19,21	1.35	2 (11%)
6	NAG	A	734	1	14,14,15	0.51	0	17,19,21	0.81	0
6	NAG	A	776	1	14,14,15	0.50	0	17,19,21	0.74	1 (5%)
6	NAG	A	762	1	14,14,15	0.50	0	17,19,21	0.90	0
6	NAG	A	741	1	14,14,15	0.53	0	17,19,21	0.84	1 (5%)
6	NAG	A	886	1	14,14,15	0.51	0	17,19,21	0.81	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
6	NAG	A	892	1	-	0/6/23/26	0/1/1/1
6	NAG	A	948	1	1/1/5/7	1/6/23/26	0/1/1/1
6	NAG	A	897	1	-	3/6/23/26	0/1/1/1
6	NAG	A	730	1	-	3/6/23/26	0/1/1/1
6	NAG	A	588	1	-	2/6/23/26	0/1/1/1
6	NAG	A	734	1	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	A	776	1	-	2/6/23/26	0/1/1/1
6	NAG	A	762	1	-	2/6/23/26	0/1/1/1
6	NAG	A	741	1	-	2/6/23/26	0/1/1/1
6	NAG	A	886	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	588	NAG	C1-O5-C5	4.26	117.96	112.19
6	A	892	NAG	C1-O5-C5	2.71	115.86	112.19
6	A	948	NAG	C1-O5-C5	2.61	115.73	112.19
6	A	588	NAG	O5-C1-C2	2.42	115.10	111.29
6	A	892	NAG	O5-C1-C2	2.18	114.74	111.29
6	A	730	NAG	C1-O5-C5	2.08	115.01	112.19
6	A	776	NAG	C1-O5-C5	2.01	114.92	112.19
6	A	741	NAG	C1-O5-C5	2.01	114.92	112.19

All (2) chirality outliers are listed below:

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

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	897	NAG	C3-C2-N2-C7
6	A	897	NAG	C8-C7-N2-C2
6	A	897	NAG	O7-C7-N2-C2
6	A	588	NAG	C8-C7-N2-C2
6	A	588	NAG	O7-C7-N2-C2
6	A	734	NAG	C1-C2-N2-C7
6	A	734	NAG	C8-C7-N2-C2
6	A	734	NAG	O7-C7-N2-C2
6	A	741	NAG	C8-C7-N2-C2
6	A	741	NAG	O7-C7-N2-C2
6	A	886	NAG	C8-C7-N2-C2
6	A	886	NAG	O7-C7-N2-C2
6	A	776	NAG	C8-C7-N2-C2
6	A	762	NAG	O5-C5-C6-O6
6	A	730	NAG	C8-C7-N2-C2
6	A	730	NAG	O7-C7-N2-C2
6	A	776	NAG	O7-C7-N2-C2
6	A	730	NAG	O5-C5-C6-O6
6	A	762	NAG	C4-C5-C6-O6
6	A	948	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
6	A	730	NAG	2	0
6	A	734	NAG	1	0
6	A	776	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	353/357 (98%)	0.01	2 (0%) 89 81	68, 98, 161, 262	0
2	C	184/184 (100%)	0.24	3 (1%) 72 59	86, 121, 182, 234	0
3	L	209/209 (100%)	0.63	18 (8%) 10 9	105, 173, 260, 460	0
4	H	220/220 (100%)	0.73	34 (15%) 2 2	95, 164, 306, 365	0
All	All	966/970 (99%)	0.35	57 (5%) 22 16	68, 124, 257, 460	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	183	THR	8.6
4	H	131	THR	7.3
4	H	194	TYR	7.2
4	H	139	GLY	6.4
4	H	138	LEU	6.4
4	H	132	SER	5.9
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	4.0
4	H	213	PRO	3.8
3	L	114	SER	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
4	H	210	LYS	3.0
3	L	185	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
4	H	128	SER	2.9
4	H	125	ALA	2.9
4	H	133	GLY	2.8
4	H	180	SER	2.8
4	H	207	VAL	2.8
3	L	155	GLN	2.7
4	H	140	CYS	2.6
2	C	1098	PHE	2.6
3	L	115	VAL	2.6
4	H	195	ILE	2.6
3	L	195	GLU	2.5
3	L	117	ILE	2.5
4	H	187	SER	2.4
3	L	145	LYS	2.4
1	A	61	TYR	2.4
4	H	191	THR	2.3
4	H	123	PRO	2.3
3	L	180	THR	2.3
2	C	1178	ALA	2.2
3	L	183	LYS	2.2
3	L	181	LEU	2.2
4	H	135	THR	2.2
4	H	190	GLY	2.2
4	H	122	PHE	2.2
3	L	118	PHE	2.2
3	L	113	PRO	2.2
4	H	129	LYS	2.1
1	A	474	ASP	2.1
4	H	124	LEU	2.1
4	H	152	VAL	2.1
4	H	185	PRO	2.1
3	L	136	LEU	2.0
4	H	208	ASP	2.0
2	C	1142	LYS	2.0
3	L	110	VAL	2.0
4	H	141	LEU	2.0

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

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

6.3 Carbohydrates [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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FUL	B	2	10/11	0.51	0.40	197,211,231,236	0
5	NAG	B	1	14/15	0.90	0.17	84,111,141,166	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	A	897	14/15	0.65	0.53	139,208,226,240	0
6	NAG	A	741	14/15	0.66	0.43	215,224,236,239	0
6	NAG	A	730	14/15	0.73	0.52	232,249,275,286	0
6	NAG	A	948	14/15	0.77	0.32	134,155,186,195	0
6	NAG	A	588	14/15	0.80	0.26	95,145,161,167	0
6	NAG	A	892	14/15	0.82	0.29	102,144,192,206	0
6	NAG	A	776	14/15	0.84	0.24	112,131,168,180	0
6	NAG	A	886	14/15	0.85	0.32	75,115,154,164	0
6	NAG	A	734	14/15	0.86	0.23	145,167,194,207	0
6	NAG	A	762	14/15	0.93	0.23	75,80,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.