



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:50 AM GMT

PDB ID : 3JVF
Title : Crystal structure of an Interleukin-17 receptor complex
Authors : Ely, L.K.; Garcia, K.C.
Deposited on : 2009-09-16
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

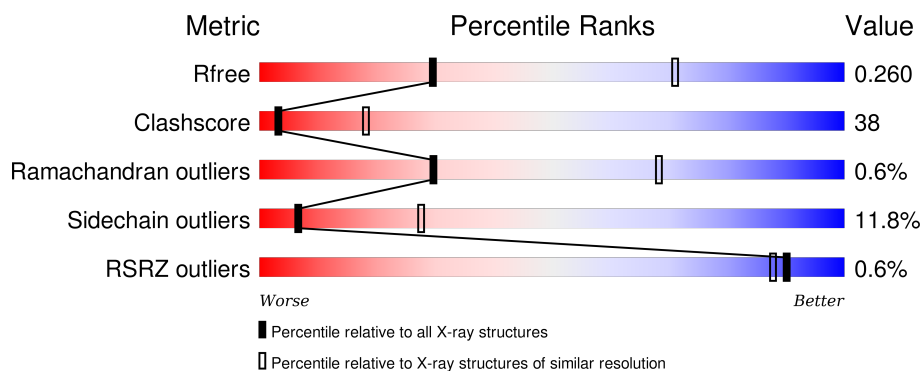
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	133	<div> <div>%</div> <div> <div></div> <div>36%</div> <div>37%</div> <div>5%</div> <div>22%</div> </div> </div>
1	B	133	<div> <div>%</div> <div> <div></div> <div>45%</div> <div>31%</div> <div>•</div> <div>22%</div> </div> </div>
2	C	286	<div> <div></div> <div> <div>36%</div> <div>49%</div> <div>10%</div> <div>5%</div> </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
4	NAG	C	302	X	-	-	-
4	NAG	C	304	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3878 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 Interleukin-17F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			795	494	144	150	7			
1	B	104	Total	C	N	O	S	0	0	0
			791	488	145	151	7			

- Molecule 2 is a protein called Interleukin-17 receptor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	271	Total	C	N	O	S	0	0	0
			2193	1382	403	393	15			

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 1: Interleukin-17F



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	170.73Å 170.73Å 81.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.82 – 3.30 39.82 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.82-3.30) 98.6 (39.82-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_162)	Depositor
R, R_{free}	0.229 , 0.256 0.224 , 0.260	Depositor DCC
R_{free} test set	947 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	96.8	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 18482 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3878	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: CA, MLY, 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	0.65	3/807 (0.4%)	0.63	0/1100
1	B	0.41	0/803	0.58	0/1094
2	C	0.40	0/2249	0.58	0/3069
All	All	0.46	3/3859 (0.1%)	0.59	0/5263

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	GLU	CD-OE1	9.16	1.35	1.25
1	A	96	GLU	CD-OE2	7.27	1.33	1.25
1	A	96	GLU	CG-CD	6.99	1.62	1.51

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	A	795	0	763	64	0
1	B	791	0	760	56	0
2	C	2193	0	2063	195	0
3	A	28	0	25	0	0
4	C	70	0	65	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
All	All	3878	0	3676	284	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 38.

All (284) 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)
2:C:124:GLN:HE21	2:C:124:GLN:HA	1.06	1.17
2:C:124:GLN:NE2	2:C:124:GLN:HA	1.73	1.03
2:C:175:ASN:HB2	2:C:232:ARG:HH12	1.20	1.02
2:C:156:HIS:HB3	2:C:159:MET:CB	1.99	0.92
2:C:43:MLY:HH21	2:C:71:THR:HG22	1.51	0.92
2:C:156:HIS:HB3	2:C:159:MET:HB2	1.50	0.91
1:A:62:ARG:NH2	1:A:67:VAL:HG12	1.84	0.90
2:C:162:THR:HG23	2:C:164:PRO:HD2	1.54	0.87
2:C:10:LEU:HB2	2:C:21:VAL:HG21	1.53	0.87
1:A:30:GLY:HA2	1:B:112:GLN:HB2	1.56	0.87
1:A:25:MET:HG3	1:B:111:PHE:HE2	1.40	0.87
2:C:260:LEU:O	2:C:261:ASN:HB3	1.75	0.86
2:C:106:HIS:HD2	2:C:108:HIS:H	1.18	0.86
2:C:175:ASN:HB2	2:C:232:ARG:NH1	1.90	0.85
1:A:62:ARG:HH21	1:A:67:VAL:HG12	1.36	0.85
2:C:124:GLN:CA	2:C:124:GLN:HE21	1.89	0.85
2:C:165:CYS:O	2:C:169:GLY:HA2	1.75	0.85
2:C:88:LEU:HD23	2:C:125:GLU:O	1.78	0.84
2:C:174:PRO:HA	2:C:191:THR:HG23	1.62	0.82
2:C:171:LEU:HD12	2:C:171:LEU:H	1.44	0.82
2:C:4:LEU:HD12	2:C:4:LEU:H	1.43	0.81
1:A:62:ARG:NH2	1:A:67:VAL:CG1	2.43	0.81
2:C:43:MLY:CH2	2:C:71:THR:HG22	2.11	0.80
2:C:7:HIS:CD2	4:C:305:NAG:H81	2.16	0.79
1:A:114:GLU:HG2	1:B:32:ILE:H	1.47	0.78
2:C:106:HIS:CD2	2:C:108:HIS:H	2.01	0.78
1:B:102:ARG:O	1:B:102:ARG:HG3	1.84	0.77
2:C:120:VAL:HG11	2:C:151:VAL:HG21	1.67	0.76
1:A:91:VAL:HG23	1:A:92:PRO:HD2	1.68	0.76
1:A:57:THR:OG1	1:A:67:VAL:HG13	1.85	0.76
2:C:54:THR:HG22	2:C:55:GLN:H	1.49	0.75
2:C:87:GLN:HB2	2:C:126:TYR:CE1	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:MET:HG3	1:B:111:PHE:CE2	2.22	0.74
2:C:19:CYS:HB2	2:C:99:GLU:O	1.87	0.74
2:C:136:PRO:HD3	2:C:143:ASN:ND2	2.01	0.74
1:B:42:ARG:HB3	1:B:42:ARG:HH11	1.52	0.74
2:C:6:ASP:HB3	2:C:8:ARG:HG2	1.68	0.74
1:B:102:ARG:HA	1:B:111:PHE:HB3	1.71	0.73
2:C:172:TRP:CZ2	2:C:174:PRO:HG3	2.24	0.72
2:C:204:THR:HG22	2:C:216:GLU:HG3	1.70	0.72
1:B:45:GLU:HG2	1:B:54:TYR:CE2	2.23	0.72
1:A:31:ILE:HG22	1:A:34:GLU:CB	2.19	0.72
1:A:63:TYR:CD1	1:A:64:PRO:HA	2.25	0.72
1:B:58:TRP:CH2	1:B:60:PRO:HG3	2.25	0.71
1:B:111:PHE:CZ	2:C:32:ILE:HG22	2.25	0.71
2:C:207:PRO:HD2	2:C:212:HIS:O	1.90	0.70
1:A:62:ARG:HH21	1:A:67:VAL:CG1	2.02	0.69
2:C:260:LEU:HD12	2:C:260:LEU:O	1.92	0.69
1:A:62:ARG:O	1:A:65:SER:HA	1.92	0.69
2:C:187:ARG:HH22	2:C:234:ASN:ND2	1.89	0.68
1:A:28:ASP:HB2	1:B:112:GLN:HB3	1.74	0.68
2:C:156:HIS:HB3	2:C:159:MET:HB3	1.74	0.67
2:C:208:HIS:HB2	2:C:246:CYS:SG	2.35	0.67
1:B:77:CYS:C	1:B:78:ILE:HD12	2.14	0.67
2:C:6:ASP:CB	2:C:8:ARG:HG2	2.25	0.67
2:C:5:LEU:CD1	2:C:5:LEU:H	2.09	0.66
2:C:87:GLN:HB2	2:C:126:TYR:HE1	1.61	0.65
2:C:137:ILE:H	2:C:137:ILE:HD13	1.61	0.65
1:A:132:VAL:HG21	2:C:176:ILE:HD12	1.79	0.65
2:C:120:VAL:CG1	2:C:151:VAL:HG21	2.26	0.65
2:C:75:ILE:HD12	2:C:107:HIS:CE1	2.32	0.65
1:A:100:VAL:HA	1:A:113:LEU:HA	1.78	0.65
2:C:162:THR:HG22	2:C:165:CYS:SG	2.37	0.65
2:C:50:HIS:HD2	2:C:64:HIS:CB	2.10	0.65
1:A:97:THR:HG23	1:A:116:VAL:HG13	1.80	0.64
1:A:30:GLY:CA	1:B:112:GLN:HB2	2.26	0.64
2:C:130:VAL:O	2:C:130:VAL:HG22	1.97	0.63
2:C:43:MLY:HH21	2:C:71:THR:CG2	2.27	0.63
1:A:96:GLU:HB2	2:C:92:GLU:HG2	1.81	0.63
1:B:38:VAL:HG12	1:B:38:VAL:O	1.98	0.63
2:C:38:THR:HG21	2:C:136:PRO:HA	1.81	0.62
1:B:102:ARG:HB2	1:B:111:PHE:CD1	2.36	0.61
1:B:42:ARG:NH1	1:B:42:ARG:HB3	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:LEU:HD12	2:C:77:TYR:CE1	2.36	0.61
1:A:69:GLN:NE2	1:A:118:VAL:HA	2.15	0.61
2:C:5:LEU:HD13	2:C:5:LEU:N	2.17	0.60
2:C:172:TRP:CH2	2:C:174:PRO:HG3	2.37	0.60
1:A:97:THR:HG22	1:A:116:VAL:O	2.02	0.60
1:B:104:HIS:CD2	2:C:138:PRO:HB3	2.37	0.60
2:C:87:GLN:O	2:C:90:THR:O	2.21	0.59
1:B:111:PHE:CZ	2:C:32:ILE:CG2	2.84	0.59
1:B:36:GLN:HA	1:B:36:GLN:OE1	2.02	0.59
2:C:41:SER:OG	2:C:143:ASN:HA	2.03	0.58
1:A:38:VAL:HG12	1:A:40:MET:H	1.68	0.58
2:C:96:VAL:HG22	2:C:97:ARG:H	1.69	0.58
1:B:63:TYR:HB3	1:B:100:VAL:CG1	2.34	0.58
1:B:102:ARG:HB2	1:B:111:PHE:HD1	1.69	0.58
1:B:88:MET:CE	1:B:126:THR:HG22	2.34	0.58
2:C:174:PRO:O	2:C:176:ILE:HG13	2.04	0.58
1:A:113:LEU:HD12	1:A:113:LEU:H	1.69	0.58
2:C:156:HIS:CD2	2:C:158:ARG:HG3	2.39	0.57
2:C:206:PHE:CE1	2:C:213:SER:HB3	2.39	0.57
2:C:264:LEU:O	2:C:264:LEU:HD12	2.04	0.57
2:C:88:LEU:N	2:C:88:LEU:HD22	2.19	0.57
1:B:68:VAL:H	2:C:91:ASN:HD21	1.51	0.57
2:C:39:PRO:HD3	2:C:134:PRO:HD2	1.87	0.56
2:C:104:LEU:H	2:C:104:LEU:HD12	1.67	0.56
2:C:191:THR:HA	2:C:232:ARG:HA	1.86	0.56
1:B:88:MET:HE1	1:B:126:THR:HG22	1.85	0.56
2:C:261:ASN:O	2:C:261:ASN:ND2	2.39	0.56
2:C:253:GLN:OE1	2:C:265:ARG:NH2	2.38	0.56
2:C:163:THR:HB	2:C:164:PRO:HD3	1.88	0.56
2:C:226:PRO:HA	2:C:229:PHE:CE2	2.40	0.56
2:C:192:LEU:HD23	2:C:192:LEU:N	2.20	0.55
2:C:185:GLN:HG2	2:C:238:THR:HG22	1.86	0.55
2:C:253:GLN:NE2	2:C:255:PHE:CZ	2.73	0.55
2:C:192:LEU:H	2:C:192:LEU:HD23	1.72	0.55
2:C:192:LEU:HD21	2:C:231:GLN:O	2.07	0.55
1:B:79:ASN:HD21	1:B:81:GLN:HB2	1.71	0.55
2:C:94:LEU:HG	2:C:118:PHE:CE1	2.41	0.55
1:A:88:MET:HA	1:A:127:PRO:HD3	1.89	0.55
2:C:136:PRO:HD3	2:C:143:ASN:HD21	1.70	0.55
1:A:55:THR:O	1:A:68:VAL:HA	2.07	0.55
2:C:32:ILE:HG13	2:C:33:HIS:HD2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:207:PRO:HD3	2:C:214:CYS:SG	2.47	0.54
1:A:27:LEU:HB3	1:B:25:MET:HB3	1.89	0.54
2:C:5:LEU:H	2:C:5:LEU:HD13	1.71	0.54
2:C:186:LEU:HD23	2:C:187:ARG:N	2.23	0.54
1:B:114:GLU:HG2	1:B:116:VAL:HG13	1.88	0.54
2:C:171:LEU:HD12	2:C:171:LEU:N	2.18	0.54
1:A:96:GLU:OE2	1:A:115:LYS:HD3	2.08	0.54
2:C:2:LEU:HD22	2:C:94:LEU:HD23	1.89	0.54
2:C:39:PRO:HG3	2:C:78:LEU:HA	1.87	0.54
2:C:122:PRO:HA	2:C:159:MET:HE2	1.89	0.54
2:C:76:LEU:CD2	2:C:105:ARG:HA	2.38	0.54
2:C:208:HIS:O	2:C:209:MET:HB2	2.07	0.54
2:C:208:HIS:CD2	2:C:209:MET:HG2	2.42	0.54
2:C:54:THR:HG22	2:C:55:GLN:N	2.21	0.54
1:B:58:TRP:CZ2	1:B:60:PRO:HG3	2.43	0.54
1:B:79:ASN:ND2	1:B:81:GLN:HB2	2.23	0.54
1:A:41:SER:O	1:A:44:ILE:HG13	2.08	0.54
1:B:99:VAL:HG23	1:B:114:GLU:HB3	1.90	0.53
2:C:45:LEU:HD13	2:C:147:LYS:HB2	1.89	0.53
2:C:142:PRO:O	2:C:143:ASN:OD1	2.25	0.53
1:A:99:VAL:HG22	1:A:116:VAL:HG12	1.89	0.53
2:C:12:CYS:HB2	2:C:98:PHE:CE2	2.43	0.53
1:B:63:TYR:HB3	1:B:100:VAL:HG13	1.89	0.53
2:C:5:LEU:CD1	2:C:5:LEU:N	2.70	0.52
2:C:131:HIS:CD2	2:C:131:HIS:H	2.27	0.52
2:C:175:ASN:O	2:C:190:PHE:HA	2.09	0.52
2:C:172:TRP:HB2	2:C:193:TRP:CE3	2.44	0.52
1:B:102:ARG:CA	1:B:111:PHE:HB3	2.39	0.52
2:C:10:LEU:HB2	2:C:21:VAL:CG2	2.32	0.51
1:B:45:GLU:HG2	1:B:54:TYR:HE2	1.71	0.51
1:A:63:TYR:HA	1:A:64:PRO:C	2.31	0.51
2:C:106:HIS:CG	2:C:108:HIS:CD2	2.97	0.51
1:A:62:ARG:NH2	1:A:67:VAL:HB	2.25	0.51
2:C:166:MET:HA	2:C:171:LEU:HD13	1.92	0.51
2:C:94:LEU:HG	2:C:118:PHE:HE1	1.76	0.51
2:C:239:LEU:HD23	2:C:248:HIS:CE1	2.46	0.51
1:A:113:LEU:O	1:B:31:ILE:HG23	2.11	0.51
2:C:45:LEU:HD22	2:C:46:GLN:N	2.26	0.51
1:B:68:VAL:N	2:C:91:ASN:HD21	2.08	0.51
2:C:83:LEU:N	2:C:83:LEU:HD12	2.26	0.51
2:C:50:HIS:HD2	2:C:64:HIS:CG	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:NH2	1:A:67:VAL:CB	2.73	0.50
1:A:91:VAL:CG2	1:A:92:PRO:HD2	2.41	0.50
2:C:133:LEU:HA	2:C:134:PRO:C	2.31	0.50
2:C:69:LEU:HB2	2:C:111:TRP:HB2	1.94	0.50
2:C:184:HIS:ND1	2:C:184:HIS:N	2.59	0.50
1:A:53:ASN:O	1:A:70:ALA:HA	2.12	0.50
2:C:251:GLN:HA	2:C:266:HIS:O	2.12	0.50
2:C:174:PRO:HB3	2:C:191:THR:O	2.11	0.50
1:A:85:ASP:OD1	1:A:85:ASP:C	2.50	0.50
1:B:31:ILE:HD12	2:C:25:THR:OG1	2.11	0.50
1:A:114:GLU:HA	1:B:31:ILE:HG23	1.94	0.50
1:B:27:LEU:HD23	1:B:28:ASP:N	2.27	0.49
2:C:120:VAL:HG22	2:C:126:TYR:CE2	2.47	0.49
1:A:97:THR:CG2	1:A:116:VAL:HG13	2.41	0.49
1:A:52:TRP:CD1	1:A:70:ALA:HB1	2.47	0.49
2:C:89:ASN:ND2	2:C:124:GLN:OE1	2.45	0.49
2:C:187:ARG:NH2	2:C:234:ASN:ND2	2.60	0.49
2:C:194:ASN:HB3	2:C:230:HIS:NE2	2.27	0.49
2:C:174:PRO:O	2:C:176:ILE:CG1	2.61	0.49
1:A:58:TRP:CZ3	1:A:66:GLU:HB2	2.48	0.49
2:C:75:ILE:HG23	2:C:76:LEU:N	2.28	0.49
2:C:50:HIS:HD2	2:C:64:HIS:HB2	1.75	0.48
1:A:125:VAL:HG11	1:B:44:ILE:HB	1.95	0.48
2:C:122:PRO:HA	2:C:159:MET:CE	2.43	0.48
2:C:19:CYS:CB	2:C:100:PHE:HA	2.43	0.48
2:C:192:LEU:CD2	2:C:231:GLN:O	2.61	0.48
2:C:71:THR:HA	2:C:107:HIS:CE1	2.49	0.48
1:B:37:ARG:NH1	2:C:92:GLU:OE2	2.47	0.48
2:C:44:ASP:HB2	2:C:68:THR:HG23	1.96	0.48
1:A:25:MET:HE2	2:C:32:ILE:HG21	1.95	0.48
2:C:88:LEU:H	2:C:88:LEU:CD2	2.27	0.48
1:B:101:ARG:HH11	1:B:101:ARG:HG3	1.79	0.47
2:C:42:PRO:HB3	2:C:67:TRP:CD1	2.50	0.47
1:A:86:ILE:HG22	1:A:86:ILE:O	2.13	0.47
2:C:88:LEU:N	2:C:88:LEU:CD2	2.77	0.47
1:A:25:MET:CE	2:C:32:ILE:HG21	2.44	0.47
2:C:4:LEU:HD12	2:C:4:LEU:N	2.20	0.47
2:C:93:ARG:HB2	2:C:93:ARG:CZ	2.44	0.47
2:C:174:PRO:O	2:C:175:ASN:C	2.51	0.47
2:C:64:HIS:HA	2:C:116:SER:HB3	1.96	0.47
1:A:95:GLN:CG	1:B:120:VAL:HG13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:PHE:HB2	2:C:119:VAL:HG22	1.96	0.46
2:C:19:CYS:HB2	2:C:100:PHE:HA	1.98	0.46
2:C:66:GLU:HA	2:C:113:PHE:O	2.16	0.46
2:C:47:ILE:HD13	2:C:128:VAL:CG1	2.45	0.46
1:A:27:LEU:HD23	1:B:27:LEU:HB2	1.98	0.46
2:C:254:PRO:HB2	2:C:256:PHE:CE1	2.51	0.46
1:B:55:THR:CB	1:B:71:GLN:HE22	2.29	0.46
2:C:33:HIS:N	2:C:34:PRO:HD3	2.31	0.46
2:C:89:ASN:HB2	2:C:90:THR:H	1.52	0.46
1:A:85:ASP:OD1	1:A:87:SER:N	2.48	0.46
2:C:166:MET:HA	2:C:171:LEU:CD1	2.46	0.45
2:C:194:ASN:HA	2:C:229:PHE:CD1	2.51	0.45
2:C:2:LEU:HD23	2:C:2:LEU:HA	1.82	0.45
2:C:171:LEU:CD1	2:C:171:LEU:H	2.22	0.45
2:C:41:SER:HA	2:C:143:ASN:O	2.17	0.45
2:C:2:LEU:HD22	2:C:94:LEU:CD2	2.47	0.45
1:A:30:GLY:HA2	1:B:112:GLN:CB	2.38	0.45
2:C:17:LEU:HD21	2:C:100:PHE:CD2	2.52	0.45
1:B:41:SER:C	1:B:42:ARG:HG2	2.36	0.45
2:C:248:HIS:O	2:C:269:THR:HA	2.16	0.45
2:C:52:ALA:HB3	2:C:62:VAL:HG21	1.99	0.45
2:C:22:LYS:HD2	2:C:99:GLU:OE1	2.16	0.45
2:C:41:SER:HA	2:C:143:ASN:C	2.37	0.45
1:B:77:CYS:O	1:B:78:ILE:HD12	2.17	0.45
1:A:93:ILE:HG21	1:B:120:VAL:HG12	1.99	0.45
1:A:88:MET:SD	1:A:126:THR:HA	2.56	0.45
2:C:181:LEU:HD12	2:C:182:GLU:H	1.81	0.45
2:C:207:PRO:HA	2:C:244:GLY:O	2.16	0.44
1:A:59:ASP:OD1	1:A:61:ASN:N	2.51	0.44
2:C:104:LEU:N	2:C:104:LEU:HD12	2.33	0.44
2:C:75:ILE:CG2	2:C:76:LEU:N	2.80	0.44
2:C:37:LEU:HD12	2:C:77:TYR:HE1	1.81	0.44
2:C:185:GLN:CG	2:C:238:THR:HG22	2.47	0.44
2:C:258:SER:O	2:C:259:CYS:SG	2.75	0.44
2:C:181:LEU:CD1	2:C:182:GLU:H	2.31	0.44
2:C:43:MLY:HB2	2:C:70:GLN:HG3	2.00	0.44
1:A:93:ILE:CG2	1:B:120:VAL:HG12	2.48	0.44
2:C:24:SER:C	2:C:25:THR:O	2.55	0.43
2:C:47:ILE:HD13	2:C:128:VAL:HG13	2.00	0.43
2:C:17:LEU:HD21	2:C:100:PHE:CE2	2.53	0.43
1:B:76:GLY:HA2	1:B:89:ASN:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:HIS:CD2	2:C:108:HIS:CD2	3.06	0.43
2:C:106:HIS:HD2	2:C:108:HIS:N	2.01	0.43
2:C:19:CYS:HB2	2:C:99:GLU:C	2.39	0.43
2:C:136:PRO:HG3	2:C:141:ASP:O	2.18	0.43
1:A:45:GLU:HB3	1:A:54:TYR:CE2	2.54	0.43
2:C:75:ILE:HB	2:C:107:HIS:HE2	1.84	0.43
2:C:65:ILE:O	2:C:114:THR:HA	2.19	0.43
1:A:25:MET:HE2	2:C:32:ILE:HD13	2.01	0.43
2:C:45:LEU:HD22	2:C:46:GLN:H	1.83	0.43
2:C:47:ILE:HD11	2:C:128:VAL:HG22	2.00	0.43
1:A:56:VAL:HG13	1:A:66:GLU:HG3	1.99	0.42
2:C:47:ILE:HD11	2:C:128:VAL:CG2	2.49	0.42
2:C:78:LEU:O	2:C:78:LEU:HD23	2.19	0.42
2:C:88:LEU:HD22	2:C:88:LEU:H	1.85	0.42
2:C:219:HIS:CE1	2:C:235:VAL:HG21	2.54	0.42
2:C:201:ILE:HD13	2:C:252:ILE:HG12	2.02	0.42
1:A:29:ILE:HG13	1:A:30:GLY:N	2.33	0.42
2:C:210:GLU:HG2	2:C:212:HIS:H	1.85	0.42
2:C:258:SER:O	2:C:259:CYS:CB	2.66	0.42
2:C:43:MLY:HH23	2:C:43:MLY:HD2	1.69	0.42
2:C:86:LEU:HG	2:C:93:ARG:HG2	2.01	0.42
2:C:3:ARG:HH11	2:C:3:ARG:HG3	1.84	0.42
1:A:48:SER:HA	1:B:124:CYS:O	2.20	0.42
1:A:42:ARG:O	1:A:43:ASN:HB2	2.19	0.42
2:C:86:LEU:HG	2:C:93:ARG:CG	2.49	0.42
2:C:229:PHE:O	2:C:230:HIS:HB2	2.20	0.41
2:C:186:LEU:HD23	2:C:187:ARG:H	1.85	0.41
2:C:22:LYS:O	2:C:23:ASN:C	2.58	0.41
2:C:6:ASP:OD2	2:C:8:ARG:NE	2.39	0.41
2:C:19:CYS:HB3	2:C:100:PHE:HD2	1.86	0.41
2:C:115:PHE:C	2:C:115:PHE:CD2	2.93	0.41
1:A:57:THR:O	1:A:67:VAL:HG13	2.21	0.41
1:B:27:LEU:HD23	1:B:27:LEU:C	2.41	0.41
1:B:88:MET:HE3	1:B:126:THR:HA	2.03	0.41
1:A:128:VAL:HG23	2:C:264:LEU:HB3	2.03	0.41
2:C:115:PHE:CE2	2:C:118:PHE:CE2	3.08	0.41
1:A:44:ILE:HG22	1:A:52:TRP:CH2	2.56	0.41
2:C:29:ASP:O	2:C:32:ILE:O	2.39	0.41
1:A:93:ILE:HD12	1:B:93:ILE:HD12	2.02	0.41
2:C:106:HIS:C	2:C:106:HIS:CD2	2.94	0.41
2:C:137:ILE:H	2:C:137:ILE:CD1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:O	1:B:122:CYS:HA	2.21	0.41
1:A:25:MET:HB3	1:B:27:LEU:O	2.20	0.40
1:A:45:GLU:O	1:A:51:PRO:HB3	2.21	0.40
2:C:137:ILE:N	2:C:137:ILE:HD13	2.32	0.40
2:C:156:HIS:O	2:C:157:ALA:C	2.59	0.40
2:C:42:PRO:HD3	2:C:143:ASN:O	2.21	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	100/133 (75%)	95 (95%)	5 (5%)	0	100	100
1	B	102/133 (77%)	96 (94%)	6 (6%)	0	100	100
2	C	268/286 (94%)	240 (90%)	25 (9%)	3 (1%)	17	57
All	All	470/552 (85%)	431 (92%)	36 (8%)	3 (1%)	30	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	89	ASN
2	C	261	ASN
2	C	174	PRO

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	89/123 (72%)	83 (93%)	6 (7%)	20	58
1	B	88/123 (72%)	82 (93%)	6 (7%)	20	57
2	C	246/270 (91%)	208 (85%)	38 (15%)	3	16
All	All	423/516 (82%)	373 (88%)	50 (12%)	6	27

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	44	ILE
1	A	65	SER
1	A	67	VAL
1	A	113	LEU
1	A	116	VAL
1	B	33	ASN
1	B	42	ARG
1	B	62	ARG
1	B	86	ILE
1	B	102	ARG
1	B	111	PHE
2	C	2	LEU
2	C	4	LEU
2	C	5	LEU
2	C	19	CYS
2	C	35	ARG
2	C	45	LEU
2	C	58	ASP
2	C	59	LEU
2	C	68	THR
2	C	70	GLN
2	C	71	THR
2	C	78	LEU
2	C	86	LEU
2	C	88	LEU
2	C	89	ASN
2	C	104	LEU
2	C	114	THR
2	C	117	HIS
2	C	124	GLN
2	C	127	GLU

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Mol	Chain	Res	Type
2	C	129	THR
2	C	130	VAL
2	C	137	ILE
2	C	158	ARG
2	C	162	THR
2	C	173	ASP
2	C	180	THR
2	C	181	LEU
2	C	184	HIS
2	C	185	GLN
2	C	188	VAL
2	C	191	THR
2	C	214	CYS
2	C	236	THR
2	C	245	CYS
2	C	259	CYS
2	C	264	LEU
2	C	269	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	43	ASN
1	B	71	GLN
1	B	74	ASN
1	B	104	HIS
2	C	7	HIS
2	C	33	HIS
2	C	46	GLN
2	C	50	HIS
2	C	55	GLN
2	C	70	GLN
2	C	91	ASN
2	C	106	HIS
2	C	108	HIS
2	C	117	HIS
2	C	131	HIS
2	C	144	HIS
2	C	145	GLN
2	C	156	HIS
2	C	198	HIS

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Mol	Chain	Res	Type
2	C	208	HIS
2	C	261	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	MLY	C	43	2	9,10,11	0.53	0	9,11,13	2.09	3 (33%)

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
2	MLY	C	43	2	-	0/7/9/11	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	43	MLY	CH2-NZ-CE	-3.96	95.02	110.79
2	C	43	MLY	O-C-CA	-3.14	117.31	125.49
2	C	43	MLY	CH2-NZ-CH1	-2.23	103.76	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	43	MLY	5	0

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$
3	NAG	A	201	1,3	14,14,15	0.63	0	15,19,21	3.33	7 (46%)
3	NAG	A	202	3	14,14,15	0.69	0	15,19,21	1.88	2 (13%)

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
3	NAG	A	201	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	202	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	NAG	C1-O5-C5	-5.28	105.54	112.25
3	A	201	NAG	O4-C4-C5	-2.34	103.05	109.24
3	A	201	NAG	O5-C5-C6	-2.22	102.53	107.35
3	A	201	NAG	O4-C4-C3	-2.09	105.62	110.34
3	A	201	NAG	C3-C2-N2	-2.00	105.76	110.56
3	A	201	NAG	C4-C3-C2	2.57	115.23	111.23
3	A	202	NAG	C3-C4-C5	3.79	116.80	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	NAG	C3-C4-C5	7.05	122.49	110.20
3	A	201	NAG	C1-O5-C5	9.32	124.07	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	C	301	2	14,14,15	0.48	0	15,19,21	0.73	0
4	NAG	C	302	2	14,14,15	0.48	0	15,19,21	0.96	1 (6%)
4	NAG	C	303	2	14,14,15	0.63	0	15,19,21	1.72	1 (6%)
4	NAG	C	304	2	14,14,15	0.82	0	15,19,21	2.90	3 (20%)
4	NAG	C	305	2	14,14,15	0.64	0	15,19,21	1.61	2 (13%)

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
4	NAG	C	301	2	-	0/6/23/26	0/1/1/1
4	NAG	C	302	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	303	2	-	0/6/23/26	0/1/1/1
4	NAG	C	304	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	305	2	-	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(°)	Ideal(°)
4	C	304	NAG	C1-O5-C5	-9.67	99.97	112.25
4	C	305	NAG	C2-N2-C7	-2.77	119.48	123.04
4	C	304	NAG	C2-N2-C7	-2.31	120.08	123.04
4	C	302	NAG	C1-O5-C5	2.98	116.03	112.25
4	C	304	NAG	O5-C5-C6	3.79	115.55	107.35
4	C	305	NAG	C1-O5-C5	5.02	118.61	112.25
4	C	303	NAG	C1-O5-C5	6.25	120.17	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	302	NAG	C1
4	C	304	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	305	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, 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	104/133 (78%)	0.03	1 (0%) 84 80	82, 111, 146, 158	0
1	B	104/133 (78%)	-0.19	1 (0%) 84 80	76, 104, 149, 154	0
2	C	270/286 (94%)	-0.09	1 (0%) 93 92	72, 108, 144, 162	0
All	All	478/552 (86%)	-0.08	3 (0%) 90 88	72, 108, 147, 162	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	PHE	2.1
2	C	209	MET	2.1
1	B	25	MET	2.0

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

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	MLY	C	43	11/12	0.96	0.23	-	73,76,84,89	0

6.3 Carbohydrates

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	201	14/15	0.92	0.19	-	139,151,161,166	0
3	NAG	A	202	14/15	0.86	0.38	-	165,171,175,184	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
5	CA	B	134	1/1	0.94	0.16	-	93,93,93,93	0
4	NAG	C	305	14/15	0.91	0.21	-	122,132,141,142	0
4	NAG	C	301	14/15	0.87	0.20	-	115,136,144,144	0
4	NAG	C	302	14/15	0.88	0.39	-	164,176,180,181	0
4	NAG	C	303	14/15	0.86	0.34	-	135,146,156,157	0
4	NAG	C	304	14/15	0.85	0.40	-	152,166,179,181	0

6.5 Other polymers [i](#)

There are no such residues in this entry.