



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2017 – 03:11 PM EDT

PDB ID : 3LRS  
Title : Structure of PG16, an antibody with broad and potent neutralization of HIV-1  
Authors : Pancera, M.; Kwong, P.D.  
Deposited on : unknown  
Resolution : 2.37 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

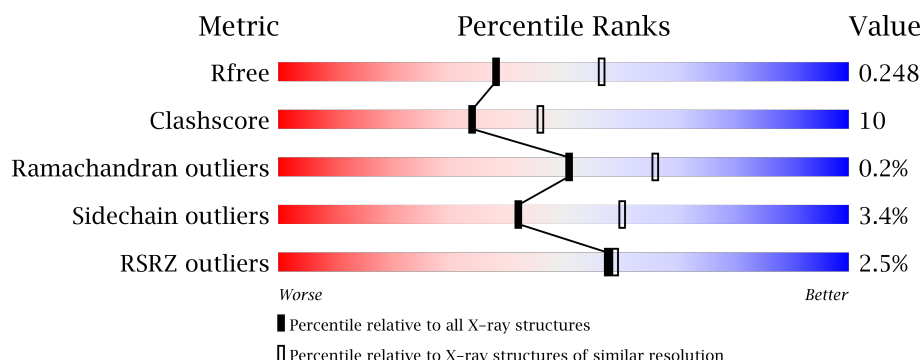
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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.



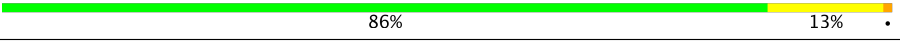


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4388 (2.40-2.36)
Clashscore	112137	4984 (2.40-2.36)
Ramachandran outliers	110173	4907 (2.40-2.36)
Sidechain outliers	110143	4909 (2.40-2.36)
RSRZ outliers	101464	4423 (2.40-2.36)

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  $\geq 3$ , 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	238	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	C	238	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>
1	E	238	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	H	238	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>• 8%</div> </div> </div>
2	B	211	<div> <div>•%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	211	
2	F	211	
2	L	211	

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
3	NAG	D	741	X	-	-	-
3	NAG	L	741	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13424 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 PG-16 Heavy Chain Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	220	Total	C	N	O	S	0	0	0
			1669	1057	284	319	9			
1	A	221	Total	C	N	O	S	0	0	0
			1675	1060	285	321	9			
1	C	228	Total	C	N	O	S	0	0	0
			1725	1089	294	333	9			
1	E	221	Total	C	N	O	S	0	0	0
			1680	1063	285	323	9			

- Molecule 2 is a protein called PG-16 Light Chain Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1558	969	264	320	5			
2	B	211	Total	C	N	O	S	0	0	0
			1558	969	264	320	5			
2	D	211	Total	C	N	O	S	0	0	0
			1557	969	264	319	5			
2	F	211	Total	C	N	O	S	0	0	0
			1557	969	264	319	5			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



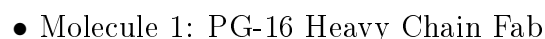
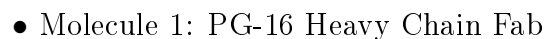
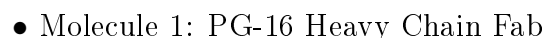
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

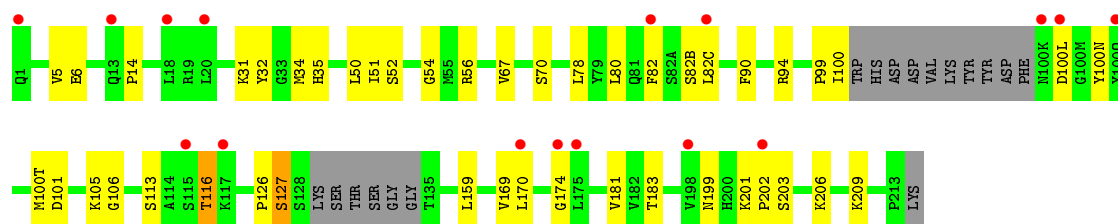
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	52	Total	O	0	0
			52	52		
4	L	46	Total	O	0	0
			46	46		
4	A	44	Total	O	0	0
			44	44		
4	B	38	Total	O	0	0
			38	38		
4	C	22	Total	O	0	0
			22	22		
4	D	73	Total	O	0	0
			73	73		
4	E	38	Total	O	0	0
			38	38		
4	F	76	Total	O	0	0
			76	76		

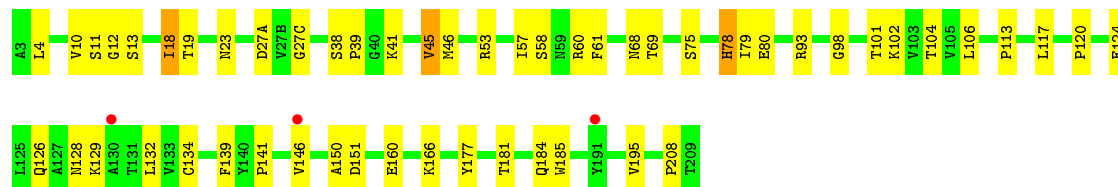
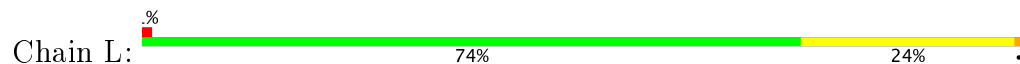


- Molecule 1: PG-16 Heavy Chain Fab

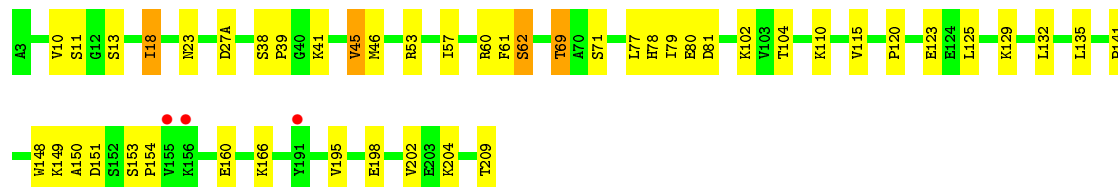
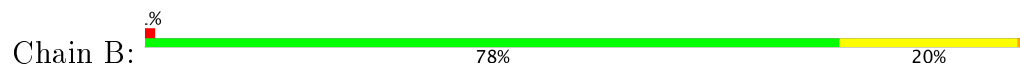




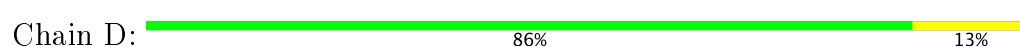
• Molecule 2: PG-16 Light Chain Fab



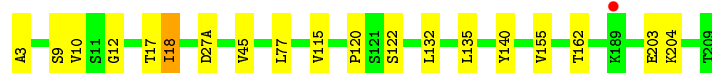
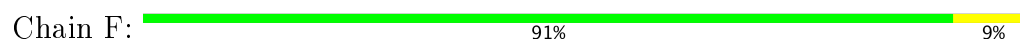
• Molecule 2: PG-16 Light Chain Fab



• Molecule 2: PG-16 Light Chain Fab



• Molecule 2: PG-16 Light Chain Fab



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.32Å 165.09Å 81.36Å 90.00° 91.55° 90.00°	Depositor
Resolution (Å)	30.59 – 2.37 30.59 – 2.37	Depositor EDS
% Data completeness (in resolution range)	82.0 (30.59-2.37) 81.9 (30.59-2.37)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.36Å)	Xtriage
Refinement program	PHENIX 1.5 _2	Depositor
R, $R_{free}$	0.211 , 0.260 0.192 , 0.248	Depositor DCC
$R_{free}$ test set	3596 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 31.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.067 for l,k,-h 0.069 for h,-k,-l 0.430 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13424	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	0/1718	0.56	0/2332
1	C	0.39	0/1769	0.58	0/2402
1	E	0.38	0/1723	0.56	0/2341
1	H	0.40	0/1712	0.57	0/2324
2	B	0.39	0/1595	0.55	0/2171
2	D	0.40	0/1594	0.58	0/2171
2	F	0.41	0/1594	0.57	0/2171
2	L	0.39	0/1595	0.56	0/2171
All	All	0.39	0/13300	0.57	0/18083

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1675	0	1627	31	0
1	C	1725	0	1677	44	0
1	E	1680	0	1627	35	0
1	H	1669	0	1622	41	0
2	B	1558	0	1507	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1557	0	1507	29	0
2	F	1557	0	1507	15	0
2	L	1558	0	1507	48	0
3	B	14	0	13	0	0
3	D	14	0	13	0	0
3	F	14	0	13	0	0
3	L	14	0	13	0	0
4	A	44	0	0	0	0
4	B	38	0	0	4	0
4	C	22	0	0	1	0
4	D	73	0	0	1	0
4	E	38	0	0	0	0
4	F	76	0	0	1	0
4	H	52	0	0	5	0
4	L	46	0	0	2	0
All	All	13424	0	12633	247	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 10.

All (247) 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:L:166:LYS:HE2	2:D:92:ASP:O	1.77	0.85
1:C:135:THR:CG2	1:C:183:THR:HG23	2.07	0.84
2:F:18:ILE:HD12	2:F:77:LEU:HD11	1.59	0.82
1:C:129:LYS:HB2	1:C:130:SER:C	2.03	0.79
1:E:99:PRO:O	1:E:100:ILE:HB	1.85	0.74
1:H:116:THR:HG22	1:H:203:SER:HB3	1.71	0.72
1:C:70:SER:O	1:C:78:LEU:HD12	1.90	0.71
2:D:18:ILE:CG2	2:D:74:ILE:HB	2.19	0.71
1:E:52:SER:HB3	1:E:56:ARG:HB3	1.74	0.68
1:E:70:SER:O	1:E:78:LEU:HD12	1.94	0.68
1:H:101:ASP:HA	2:L:45:VAL:HG21	1.76	0.67
1:C:181:VAL:HG11	2:D:135:LEU:CD1	2.24	0.67
2:L:104:THR:HG23	4:L:214:HOH:O	1.96	0.66
1:C:129:LYS:HB3	1:C:131:THR:OG1	1.95	0.66
1:H:89:MET:HE2	1:H:108:THR:HG22	1.77	0.65
1:C:129:LYS:HB2	1:C:130:SER:CA	2.27	0.64
2:L:10:VAL:HG13	2:L:101:THR:HG21	1.79	0.64
1:C:186:SER:HA	1:C:189:LEU:HD23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:LYS:HB3	1:C:131:THR:HG23	1.80	0.64
1:H:115:SER:HA	4:H:244:HOH:O	1.98	0.63
2:L:120:PRO:HD3	2:L:132:LEU:CD2	2.27	0.62
1:H:100(T):MET:O	2:L:45:VAL:HG22	2.00	0.62
1:E:116:THR:HG21	1:E:202:PRO:O	2.00	0.62
2:L:11:SER:C	2:L:18:ILE:HD11	2.19	0.61
2:B:209:THR:HA	4:B:227:HOH:O	1.98	0.61
1:A:178:LEU:HD12	1:A:178:LEU:C	2.20	0.61
1:C:129:LYS:HB3	1:C:131:THR:CG2	2.30	0.61
1:H:12:VAL:HG23	1:H:111:VAL:HG22	1.84	0.60
1:A:162:GLY:O	1:A:182:VAL:HA	2.02	0.60
2:D:18:ILE:HG22	2:D:74:ILE:O	2.02	0.60
2:B:120:PRO:HD3	2:B:132:LEU:CD2	2.33	0.59
1:C:199:ASN:ND2	1:C:206:LYS:HE2	2.18	0.59
2:B:104:THR:HG21	2:B:141:PRO:HB3	1.85	0.59
2:D:41:LYS:HD3	2:D:42:ALA:H	1.68	0.58
1:A:13:GLN:OE1	1:A:113:SER:HA	2.03	0.58
1:C:135:THR:HG21	1:C:183:THR:HG23	1.83	0.58
2:L:78:HIS:HB3	2:L:80:GLU:OE2	2.04	0.58
2:B:11:SER:C	2:B:18:ILE:HD11	2.23	0.58
2:L:185:TRP:CZ2	2:L:208:PRO:HA	2.39	0.58
2:B:11:SER:O	2:B:18:ILE:HD11	2.03	0.58
2:L:60:ARG:HD2	2:L:75:SER:O	2.04	0.58
2:L:46:MET:HA	2:L:57:ILE:HD13	1.85	0.58
1:A:178:LEU:HD12	1:A:179:SER:N	2.18	0.57
1:H:159:LEU:HD12	4:H:250:HOH:O	2.04	0.57
1:A:101:ASP:HA	2:B:45:VAL:HG21	1.87	0.56
1:H:129:LYS:HE2	1:H:136:ALA:HA	1.86	0.56
2:L:23:ASN:ND2	2:L:69:THR:HG21	2.20	0.56
1:C:6:GLU:OE1	1:C:105:LYS:O	2.24	0.56
1:E:199:ASN:ND2	1:E:206:LYS:HE2	2.21	0.56
1:H:23:LEU:C	1:H:23:LEU:HD23	2.27	0.55
1:E:35:HIS:CE1	1:E:50:LEU:HD13	2.41	0.55
2:L:10:VAL:HG13	2:L:101:THR:CG2	2.36	0.55
1:E:181:VAL:HG11	2:F:135:LEU:HD13	1.89	0.55
1:H:144:ASP:OD2	2:L:129:LYS:NZ	2.40	0.55
2:D:10:VAL:HG13	2:D:101:THR:HG21	1.89	0.55
1:A:145:TYR:CE1	1:A:150:VAL:HG23	2.42	0.54
2:B:115:VAL:HG13	2:B:202:VAL:HG11	1.89	0.54
1:A:169:VAL:HG21	2:B:160:GLU:HB3	1.89	0.54
1:A:100(T):MET:O	2:B:45:VAL:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:HG23	1:A:5:VAL:O	2.07	0.54
1:H:178:LEU:C	1:H:178:LEU:HD12	2.28	0.54
1:E:32:TYR:CG	1:E:94:ARG:HD2	2.42	0.53
1:H:183:THR:HG22	1:H:183:THR:O	2.08	0.53
1:C:135:THR:HG23	1:C:183:THR:HG23	1.88	0.53
1:E:100(T):MET:O	2:F:45:VAL:HG22	2.08	0.53
1:H:123:PRO:HG3	1:H:209:LYS:HD2	1.91	0.53
1:E:82:PHE:HB3	1:E:82(C):LEU:HD11	1.91	0.53
1:E:169:VAL:HB	2:F:162:THR:HG22	1.89	0.53
1:C:34:MET:HB3	1:C:78:LEU:HD22	1.91	0.52
1:H:169:VAL:HG11	2:L:160:GLU:HB3	1.91	0.52
1:E:181:VAL:HG11	2:F:135:LEU:CD1	2.39	0.52
2:F:120:PRO:HD3	2:F:132:LEU:HD23	1.90	0.52
2:L:102:LYS:HE2	2:L:104:THR:HG22	1.90	0.52
2:L:23:ASN:HA	2:L:69:THR:HG22	1.91	0.52
1:A:199:ASN:ND2	1:A:206:LYS:HE2	2.24	0.52
2:B:110:LYS:HD3	2:B:198:GLU:HG3	1.91	0.52
2:B:38:SER:HB3	2:B:39:PRO:HD2	1.90	0.52
1:E:52:SER:HB3	1:E:56:ARG:HE	1.74	0.52
1:A:29:PHE:CD2	1:A:76:ASN:HA	2.44	0.52
2:D:115:VAL:HG23	2:D:204:LYS:HG3	1.91	0.52
2:D:17:THR:HG22	2:D:18:ILE:N	2.24	0.52
2:L:53:ARG:HD3	2:L:61:PHE:O	2.10	0.52
2:F:203:GLU:O	2:F:204:LYS:HD3	2.08	0.51
1:H:81:GLN:HG3	1:H:82:PHE:N	2.26	0.51
1:A:181:VAL:HG11	2:B:135:LEU:CD1	2.40	0.51
2:B:38:SER:HB2	2:B:41:LYS:HD2	1.91	0.51
1:H:34:MET:HB3	1:H:78:LEU:HD22	1.93	0.51
2:B:125:LEU:HD23	2:B:129:LYS:O	2.10	0.51
2:B:46:MET:HA	2:B:57:ILE:HD13	1.93	0.50
1:H:162:GLY:O	1:H:182:VAL:HA	2.12	0.50
1:E:82:PHE:CB	1:E:82(C):LEU:HD11	2.42	0.49
1:H:116:THR:HG22	1:H:203:SER:CB	2.42	0.49
1:E:100(T):MET:O	2:F:45:VAL:CG2	2.59	0.49
1:A:6:GLU:CD	1:A:106:GLY:HA2	2.32	0.49
2:F:3:ALA:N	4:F:339:HOH:O	2.44	0.49
1:H:100(S):TYR:CE1	1:H:101:ASP:HB3	2.48	0.49
1:A:126:PRO:HG3	1:A:138:LEU:HB3	1.94	0.49
1:H:201:LYS:HB2	1:H:202:PRO:HD3	1.95	0.49
1:C:6:GLU:OE1	1:C:6:GLU:N	2.46	0.48
2:L:146:VAL:HG22	2:L:195:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:ASN:HA	2:B:69:THR:HG22	1.96	0.48
1:C:186:SER:HA	1:C:189:LEU:CD2	2.42	0.48
1:E:105:LYS:HD2	1:E:106:GLY:H	1.78	0.48
1:H:101:ASP:HA	2:L:45:VAL:CG2	2.42	0.48
1:A:34:MET:HB3	1:A:78:LEU:HD22	1.95	0.48
1:E:126:PRO:O	1:E:127:SER:HB2	2.14	0.48
1:H:178:LEU:HD12	1:H:179:SER:N	2.29	0.47
1:A:116:THR:HG22	1:A:203:SER:HB3	1.96	0.47
1:E:116:THR:HG22	1:E:203:SER:HB3	1.96	0.47
2:F:12:GLY:N	2:F:18:ILE:HD11	2.29	0.47
2:L:10:VAL:CG1	2:L:101:THR:HG21	2.43	0.47
2:L:38:SER:HB2	2:L:41:LYS:HD2	1.97	0.47
2:B:53:ARG:HD3	2:B:61:PHE:O	2.15	0.47
1:C:28:THR:CG2	1:C:30:HIS:CE1	2.98	0.47
2:L:27(C):GLY:HA3	2:L:68:ASN:OD1	2.15	0.47
1:C:201:LYS:N	1:C:202:PRO:CD	2.78	0.47
1:E:34:MET:HB3	1:E:78:LEU:HD22	1.96	0.47
2:L:117:LEU:HD13	2:L:134:CYS:HB2	1.96	0.47
1:E:6:GLU:OE1	1:E:105:LYS:O	2.33	0.47
2:L:12:GLY:N	2:L:18:ILE:HD11	2.29	0.47
1:C:107:THR:HG23	1:C:107:THR:O	2.15	0.46
2:D:17:THR:HG22	2:D:18:ILE:H	1.80	0.46
1:A:105:LYS:O	1:A:106:GLY:O	2.32	0.46
1:C:129:LYS:HB2	1:C:130:SER:HA	1.97	0.46
1:H:5:VAL:O	1:H:5:VAL:HG23	2.15	0.46
1:C:135:THR:HG21	1:C:183:THR:CG2	2.45	0.46
2:L:23:ASN:ND2	2:L:69:THR:CG2	2.78	0.46
2:B:102:LYS:HE3	4:B:334:HOH:O	2.16	0.46
2:B:18:ILE:HD12	2:B:77:LEU:HD11	1.98	0.46
2:B:115:VAL:HG22	2:B:204:LYS:HG2	1.98	0.46
2:L:106:LEU:HD21	2:L:141:PRO:HG3	1.97	0.46
2:D:10:VAL:HG13	2:D:101:THR:CG2	2.44	0.46
1:C:166:PHE:HB3	4:D:311:HOH:O	2.15	0.46
2:D:18:ILE:HG23	2:D:18:ILE:O	2.16	0.46
1:H:115:SER:C	4:H:218:HOH:O	2.54	0.46
2:B:60:ARG:NH2	2:B:81:ASP:OD2	2.46	0.46
2:L:60:ARG:HB2	2:L:75:SER:O	2.16	0.46
2:D:149:LYS:HE3	2:D:152:SER:O	2.15	0.45
1:E:201:LYS:N	1:E:202:PRO:CD	2.79	0.45
2:F:155:VAL:O	2:F:155:VAL:HG12	2.14	0.45
2:L:38:SER:HB3	2:L:39:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:HIS:HB3	2:B:80:GLU:OE2	2.15	0.45
1:C:82:PHE:HZ	1:C:90:PHE:CZ	2.33	0.45
1:C:32:TYR:CG	1:C:94:ARG:HD2	2.51	0.45
2:B:78:HIS:HB2	2:B:80:GLU:HG2	1.98	0.45
1:C:129:LYS:HB3	1:C:131:THR:CB	2.47	0.45
2:D:115:VAL:CG2	2:D:204:LYS:HG3	2.46	0.45
2:L:104:THR:HG21	4:L:229:HOH:O	2.16	0.45
1:A:100(S):TYR:CE1	1:A:101:ASP:HB3	2.52	0.45
1:H:169:VAL:HG21	2:L:177:TYR:CD2	2.51	0.45
1:C:129:LYS:CB	1:C:130:SER:C	2.81	0.45
1:C:127:SER:HA	1:C:128:SER:C	2.34	0.45
2:L:126:GLN:C	2:L:128:ASN:H	2.20	0.45
1:C:51:ILE:HG12	1:C:54:GLY:HA2	1.99	0.45
1:A:35:HIS:HE2	1:A:95:GLU:HB2	1.83	0.44
2:B:148:TRP:O	2:B:149:LYS:HG3	2.17	0.44
1:E:6:GLU:OE1	1:E:6:GLU:N	2.50	0.44
2:L:113:PRO:HB3	2:L:139:PHE:CD2	2.53	0.44
1:C:171:GLN:HG2	2:D:160:GLU:HG3	2.00	0.44
2:D:167:GLN:OE1	2:D:173:ALA:HB2	2.18	0.44
2:L:58:SER:OG	2:L:60:ARG:HG2	2.17	0.44
2:B:153:SER:HA	2:B:154:PRO:HD3	1.88	0.44
1:C:100(T):MET:O	2:D:45:VAL:CG2	2.66	0.44
2:F:120:PRO:HD3	2:F:132:LEU:CD2	2.48	0.44
2:L:195:VAL:O	2:L:195:VAL:HG23	2.18	0.44
1:E:82:PHE:HB3	1:E:82(C):LEU:CD1	2.48	0.44
1:C:139:GLY:HA2	1:C:154:TRP:CH2	2.53	0.43
2:F:140:TYR:CD1	2:F:140:TYR:C	2.91	0.43
2:D:153:SER:HA	2:D:154:PRO:HD3	1.93	0.43
1:H:4:LEU:HB3	1:H:22:CYS:SG	2.58	0.43
1:H:184:VAL:HG11	1:H:194:TYR:CE1	2.53	0.43
1:A:119:PRO:HD2	1:A:205:THR:HG21	1.99	0.43
1:A:30:HIS:O	1:A:52(A):ASP:HB2	2.18	0.43
2:D:167:GLN:O	2:D:169:ASN:O	2.36	0.43
2:B:120:PRO:HD3	2:B:132:LEU:HD21	1.99	0.43
1:H:116:THR:N	4:H:218:HOH:O	2.50	0.43
2:L:106:LEU:CD2	2:L:141:PRO:HG3	2.49	0.43
2:L:79:ILE:HD13	2:D:93:ARG:CZ	2.48	0.43
2:D:93:ARG:O	2:D:94:SER:HB2	2.19	0.42
2:B:62:SER:HB3	4:B:238:HOH:O	2.19	0.42
1:C:210:ARG:HG2	4:C:221:HOH:O	2.18	0.42
1:C:22:CYS:HB3	1:C:78:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:ASP:OD1	2:D:189:LYS:HB3	2.19	0.42
1:H:29:PHE:CD2	1:H:76:ASN:HA	2.54	0.42
1:C:100:ILE:HD12	1:C:100:ILE:HA	1.95	0.42
1:C:136:ALA:HB3	1:C:189:LEU:HD21	2.00	0.42
1:C:184:VAL:HG11	1:C:194:TYR:CE1	2.55	0.42
1:H:115:SER:N	4:H:218:HOH:O	2.53	0.42
1:A:145:TYR:CZ	1:A:150:VAL:HG23	2.54	0.42
1:A:123:PRO:HG3	1:A:209:LYS:HD2	2.02	0.42
1:E:209:LYS:HD2	1:E:209:LYS:HA	1.91	0.42
1:H:89:MET:CE	1:H:108:THR:HG22	2.45	0.42
2:L:79:ILE:CD1	2:D:93:ARG:CZ	2.97	0.42
1:C:100(T):MET:O	2:D:45:VAL:HG22	2.20	0.42
1:C:82:PHE:HZ	1:C:90:PHE:CE1	2.38	0.42
1:E:31:LYS:HD3	1:E:100(N):TYR:CZ	2.54	0.42
1:C:122:PHE:CE1	2:D:124:GLU:HA	2.55	0.42
1:E:82:PHE:HZ	1:E:90:PHE:CE1	2.38	0.42
1:E:99:PRO:O	1:E:100:ILE:CB	2.59	0.42
1:C:181:VAL:HG11	2:D:135:LEU:HD13	2.00	0.42
2:D:140:TYR:C	2:D:140:TYR:CD1	2.93	0.42
2:L:120:PRO:HD3	2:L:132:LEU:HD21	2.00	0.42
2:L:93:ARG:HG2	2:L:93:ARG:HH11	1.85	0.41
1:A:15:GLY:HA2	1:A:82(B):SER:HA	2.02	0.41
1:A:36:TRP:O	1:A:48:VAL:HB	2.20	0.41
2:B:45:VAL:O	2:B:57:ILE:CD1	2.68	0.41
2:B:150:ALA:O	2:B:151:ASP:HB2	2.20	0.41
2:D:17:THR:CG2	2:D:18:ILE:N	2.83	0.41
2:D:17:THR:CG2	2:D:18:ILE:H	2.33	0.41
1:E:105:LYS:HD2	1:E:106:GLY:N	2.35	0.41
1:H:169:VAL:HG21	2:L:177:TYR:CE2	2.56	0.41
1:H:82(A):SER:O	1:H:82(B):SER:C	2.57	0.41
1:A:101:ASP:HA	2:B:45:VAL:CG2	2.48	0.41
1:C:105:LYS:HD2	1:C:105:LYS:HA	1.74	0.41
1:C:148:GLU:HG3	1:C:149:PRO:HA	2.03	0.41
1:E:170:LEU:HD11	1:E:174:GLY:O	2.21	0.41
2:L:12:GLY:HA3	2:L:18:ILE:HD12	2.01	0.41
1:A:82(A):SER:O	1:A:82(B):SER:C	2.59	0.41
1:E:67:VAL:HB	1:E:80:LEU:HD11	2.03	0.41
1:C:99:PRO:O	1:C:100:ILE:HB	2.21	0.41
1:H:13:GLN:OE1	1:H:113:SER:HA	2.20	0.41
1:H:199:ASN:ND2	1:H:206:LYS:HE2	2.35	0.41
1:E:51:ILE:HG23	1:E:51:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:ARG:NH1	1:H:79:TYR:CE1	2.89	0.41
1:A:201:LYS:N	1:A:202:PRO:CD	2.84	0.41
2:B:13:SER:HB3	4:B:379:HOH:O	2.20	0.41
2:D:34:TRP:CE2	2:D:72:LEU:HB2	2.56	0.41
1:C:6:GLU:CD	1:C:105:LYS:O	2.60	0.41
2:L:150:ALA:O	2:L:151:ASP:HB2	2.21	0.41
1:H:169:VAL:CG1	2:L:160:GLU:HB3	2.50	0.41
1:E:100(L):ASP:N	1:E:100(L):ASP:OD1	2.54	0.40
2:F:17:THR:HG22	2:F:18:ILE:N	2.36	0.40
1:H:58:TYR:N	1:H:58:TYR:CD2	2.88	0.40
2:L:181:THR:OG1	2:L:184:GLN:HG3	2.21	0.40
1:E:51:ILE:HG12	1:E:54:GLY:HA2	2.02	0.40
1:A:100(T):MET:O	2:B:45:VAL:CG2	2.69	0.40
1:E:101:ASP:HA	2:F:45:VAL:HG21	2.01	0.40
1:E:14:PRO:HG2	1:E:113:SER:HB2	2.03	0.40
1:H:164:HIS:HB2	1:H:181:VAL:HG23	2.04	0.40
2:L:45:VAL:O	2:L:57:ILE:HD11	2.21	0.40
2:L:4:LEU:O	2:L:98:GLY:HA2	2.22	0.40
1:A:147:PRO:HD2	1:A:202:PRO:CB	2.52	0.40
1:A:5:VAL:CG2	1:A:5:VAL:O	2.70	0.40
1:H:30:HIS:O	1:H:52(A):ASP:HB2	2.21	0.40
2:B:166:LYS:HB3	2:B:166:LYS:HE2	1.92	0.40
1:H:142:VAL:HG11	1:H:150:VAL:HG11	2.03	0.40
2:L:124:GLU:HG2	2:L:129:LYS: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	215/238 (90%)	204 (95%)	10 (5%)	1 (0%)	32 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	224/238 (94%)	206 (92%)	17 (8%)	1 (0%)	38	51
1	E	215/238 (90%)	198 (92%)	16 (7%)	1 (0%)	32	44
1	H	214/238 (90%)	201 (94%)	13 (6%)	0	100	100
2	B	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
2	D	209/211 (99%)	197 (94%)	12 (6%)	0	100	100
2	F	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
2	L	209/211 (99%)	197 (94%)	12 (6%)	0	100	100
All	All	1704/1796 (95%)	1606 (94%)	95 (6%)	3 (0%)	51	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	GLY
1	E	127	SER
1	C	213	PRO

### 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	186/202 (92%)	180 (97%)	6 (3%)	44	62
1	C	192/202 (95%)	185 (96%)	7 (4%)	40	58
1	E	187/202 (93%)	182 (97%)	5 (3%)	50	68
1	H	185/202 (92%)	179 (97%)	6 (3%)	44	62
2	B	178/178 (100%)	168 (94%)	10 (6%)	25	36
2	D	178/178 (100%)	174 (98%)	4 (2%)	57	75
2	F	178/178 (100%)	172 (97%)	6 (3%)	42	60
2	L	178/178 (100%)	172 (97%)	6 (3%)	42	60
All	All	1462/1520 (96%)	1412 (97%)	50 (3%)	42	60

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

Mol	Chain	Res	Type
1	H	100(T)	MET
1	H	178	LEU
1	H	181	VAL
1	H	183	THR
1	H	191	THR
1	H	197	ASN
2	L	13	SER
2	L	18	ILE
2	L	19	THR
2	L	27(A)	ASP
2	L	45	VAL
2	L	78	HIS
1	A	17	SER
1	A	28	THR
1	A	105	LYS
1	A	178	LEU
1	A	183	THR
1	A	191	THR
2	B	10	VAL
2	B	18	ILE
2	B	27(A)	ASP
2	B	45	VAL
2	B	62	SER
2	B	69	THR
2	B	71	SER
2	B	79	ILE
2	B	123	GLU
2	B	195	VAL
1	C	5	VAL
1	C	23	LEU
1	C	52(A)	ASP
1	C	148	GLU
1	C	151	THR
1	C	183	THR
1	C	191	THR
2	D	27(A)	ASP
2	D	82	GLU
2	D	115	VAL
2	D	153	SER
1	E	5	VAL
1	E	82(B)	SER
1	E	116	THR

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Mol	Chain	Res	Type
1	E	159	LEU
1	E	183	THR
2	F	9	SER
2	F	10	VAL
2	F	18	ILE
2	F	27(A)	ASP
2	F	115	VAL
2	F	122	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	C	30	HIS
2	F	188	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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
3	NAG	B	741	2	14,14,15	0.55	0	15,19,21	2.08	3 (20%)
3	NAG	D	741	2	14,14,15	0.46	0	15,19,21	1.18	2 (13%)
3	NAG	F	741	2	14,14,15	0.54	0	15,19,21	0.96	2 (13%)
3	NAG	L	741	2	14,14,15	0.50	0	15,19,21	2.17	4 (26%)

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	B	741	2	-	0/6/23/26	0/1/1/1
3	NAG	D	741	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	F	741	2	-	0/6/23/26	0/1/1/1
3	NAG	L	741	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	741	NAG	O5-C1-C2	-5.76	103.46	111.47
3	F	741	NAG	O5-C1-C2	-2.53	107.95	111.47
3	D	741	NAG	O5-C1-C2	-2.26	108.33	111.47
3	F	741	NAG	C2-N2-C7	-2.19	119.75	122.94
3	B	741	NAG	C4-C3-C2	-2.10	107.94	111.02
3	D	741	NAG	C1-O5-C5	2.18	115.17	112.17
3	B	741	NAG	O5-C1-C2	2.32	114.70	111.47
3	L	741	NAG	C3-C4-C5	2.89	115.31	110.22
3	L	741	NAG	C1-O5-C5	2.94	116.22	112.17
3	L	741	NAG	C1-C2-N2	3.19	115.94	110.49
3	B	741	NAG	C1-O5-C5	6.90	121.67	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	741	NAG	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	221/238 (92%)	0.02	4 (1%) 69 70	40, 64, 101, 144	0
1	C	228/238 (95%)	0.34	13 (5%) 24 26	36, 66, 119, 186	0
1	E	221/238 (92%)	0.29	16 (7%) 16 17	39, 65, 108, 170	0
1	H	220/238 (92%)	0.13	4 (1%) 69 70	39, 63, 100, 127	0
2	B	211/211 (100%)	0.06	3 (1%) 75 77	37, 58, 105, 130	0
2	D	211/211 (100%)	-0.09	0 100 100	36, 53, 91, 124	0
2	F	211/211 (100%)	-0.02	1 (0%) 90 91	35, 53, 94, 109	0
2	L	211/211 (100%)	0.01	3 (1%) 75 77	38, 59, 106, 135	0
All	All	1734/1796 (96%)	0.09	44 (2%) 58 59	35, 60, 106, 186	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100(L)	ASP	5.9
1	H	100(O)	TYR	4.8
2	B	155	VAL	4.5
1	H	1	GLN	4.4
1	E	115	SER	3.5
1	E	117	LYS	3.2
1	C	100(K)	ASN	3.2
1	C	100(N)	TYR	3.1
1	C	100(O)	TYR	3.0
1	E	175	LEU	2.9
1	E	174	GLY	2.8
1	E	13	GLN	2.8
2	L	191	TYR	2.8
1	E	100(K)	ASN	2.7
1	H	83	LYS	2.7
1	E	20	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	82	PHE	2.6
1	C	1	GLN	2.6
2	F	189	LYS	2.6
1	C	18	LEU	2.6
2	B	191	TYR	2.5
1	C	132	SER	2.5
2	L	130	ALA	2.5
1	E	1	GLN	2.5
1	E	82(C)	LEU	2.5
1	H	172	SER	2.5
1	C	114	ALA	2.5
1	A	118	GLY	2.5
1	A	82	PHE	2.4
1	A	129	LYS	2.3
1	C	146	PHE	2.3
1	E	100(L)	ASP	2.3
1	C	55	MET	2.3
1	E	198	VAL	2.2
1	C	116	THR	2.2
1	C	141	LEU	2.2
1	A	83	LYS	2.2
2	B	156	LYS	2.2
1	E	202	PRO	2.2
1	E	18	LEU	2.1
1	E	100(O)	TYR	2.1
2	L	146	VAL	2.1
1	E	170	LEU	2.1
1	C	12	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](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	L	741	14/15	0.70	0.23	2.40	84,102,108,109	0
3	NAG	F	741	14/15	0.88	0.12	-	73,83,89,90	0
3	NAG	D	741	14/15	0.83	0.18	-	90,96,102,105	0
3	NAG	B	741	14/15	0.89	0.23	-	86,91,97,99	0

## 6.5 Other polymers

There are no such residues in this entry.