



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2017 – 11:12 PM EDT

PDB ID : 4IOP  
Title : Crystal structure of NKp65 bound to its ligand KACL  
Authors : Li, Y.  
Deposited on : unknown  
Resolution : 3.20 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

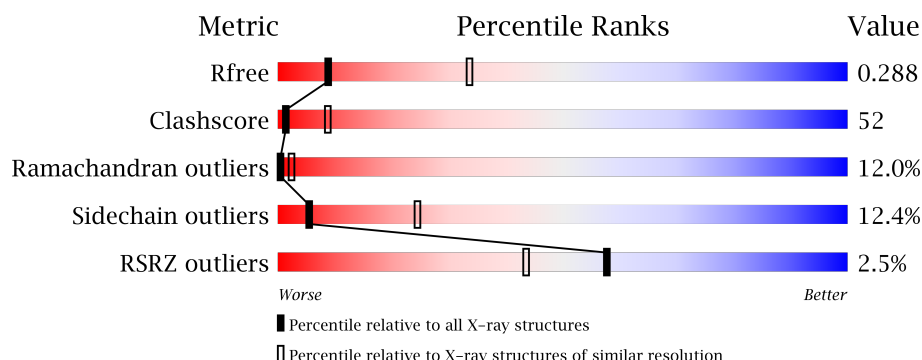
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	142	<div> <div>4%</div> <div> <div></div> <div>31%</div> <div>39%</div> <div>13%</div> <div>18%</div> </div> </div>
2	B	158	<div> <div>%</div> <div> <div></div> <div>26%</div> <div>38%</div> <div>12%</div> <div>23%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1957 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 C-type lectin domain family 2 member A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	0	0	0
			920	587	158	169	6			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ASP	-	EXPRESSION TAG	UNP Q6UVW9
A	43	LEU	-	EXPRESSION TAG	UNP Q6UVW9
A	44	GLY	-	EXPRESSION TAG	UNP Q6UVW9
A	45	SER	-	EXPRESSION TAG	UNP Q6UVW9
A	175	ALA	-	EXPRESSION TAG	UNP Q6UVW9
A	176	ALA	-	EXPRESSION TAG	UNP Q6UVW9
A	177	ALA	-	EXPRESSION TAG	UNP Q6UVW9
A	178	HIS	-	EXPRESSION TAG	UNP Q6UVW9
A	179	HIS	-	EXPRESSION TAG	UNP Q6UVW9
A	180	HIS	-	EXPRESSION TAG	UNP Q6UVW9
A	181	HIS	-	EXPRESSION TAG	UNP Q6UVW9
A	182	HIS	-	EXPRESSION TAG	UNP Q6UVW9
A	183	HIS	-	EXPRESSION TAG	UNP Q6UVW9

- Molecule 2 is a protein called Killer cell lectin-like receptor subfamily F member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			959	617	158	177	7			

There are 13 discrepancies between the modelled and reference sequences:

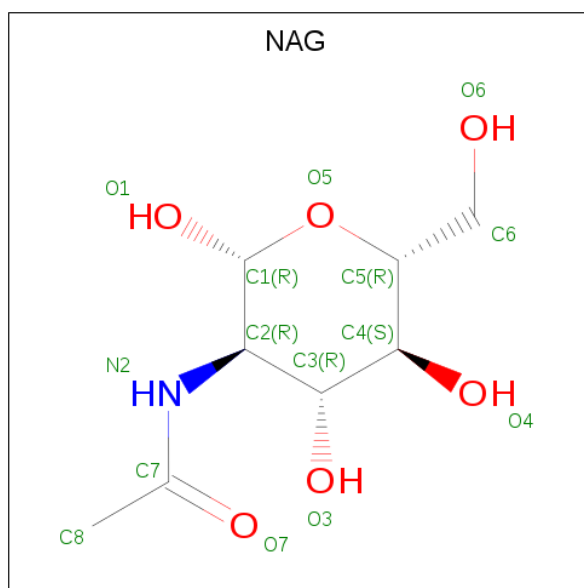
Chain	Residue	Modelled	Actual	Comment	Reference
B	59	ASP	-	EXPRESSION TAG	UNP D3W0D1
B	60	LEU	-	EXPRESSION TAG	UNP D3W0D1
B	61	GLY	-	EXPRESSION TAG	UNP D3W0D1

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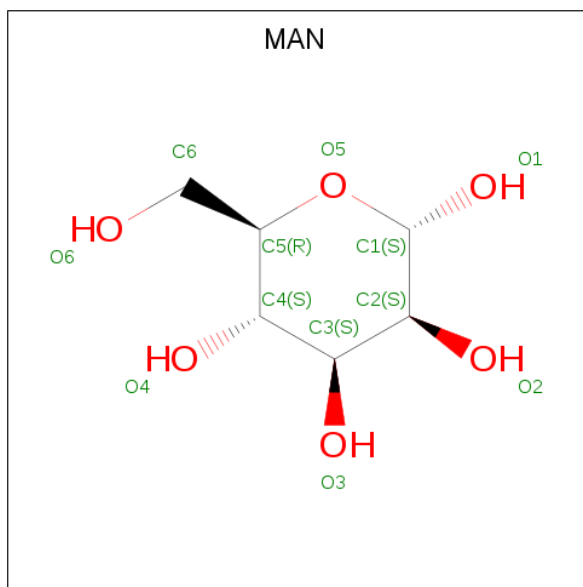
Chain	Residue	Modelled	Actual	Comment	Reference
B	62	SER	-	EXPRESSION TAG	UNP D3W0D1
B	208	ALA	-	EXPRESSION TAG	UNP D3W0D1
B	209	ALA	-	EXPRESSION TAG	UNP D3W0D1
B	210	ALA	-	EXPRESSION TAG	UNP D3W0D1
B	211	HIS	-	EXPRESSION TAG	UNP D3W0D1
B	212	HIS	-	EXPRESSION TAG	UNP D3W0D1
B	213	HIS	-	EXPRESSION TAG	UNP D3W0D1
B	214	HIS	-	EXPRESSION TAG	UNP D3W0D1
B	215	HIS	-	EXPRESSION TAG	UNP D3W0D1
B	216	HIS	-	EXPRESSION TAG	UNP D3W0D1

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

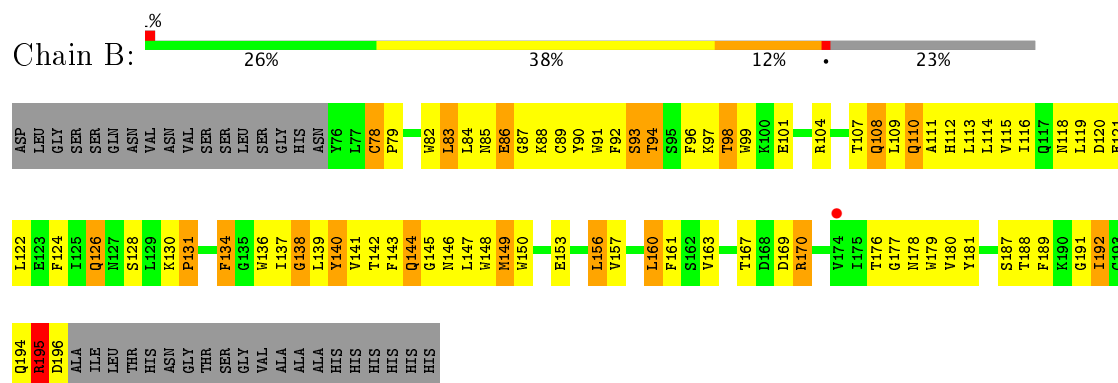
- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		



- Molecule 1: C-type lectin domain family 2 member A



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.64Å 74.64Å 271.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 71.96 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.20) 99.8 (71.96-3.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.36 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.252 , 0.297 0.270 , 0.288	Depositor DCC
$R_{free}$ test set	323 reflections (4.80%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.9	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 77.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	1957	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.47	0/947	0.69	0/1279
2	B	0.51	0/989	0.69	0/1350
All	All	0.49	0/1936	0.69	0/2629

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 ⓘ

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	920	0	836	89	0
2	B	959	0	863	114	0
3	A	56	0	48	7	0
4	A	22	0	20	0	0
All	All	1957	0	1767	194	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 52.

All (194) 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:110:GLY:HA2	1:A:151:ALA:HB2	1.35	1.03
2:B:142:THR:HG22	2:B:147:LEU:H	1.24	1.02
1:A:116:ILE:HD11	1:A:147:ALA:HB3	1.44	0.98
1:A:95:GLN:HE22	3:A:201:NAG:C6	1.80	0.93
1:A:110:GLY:HA2	1:A:151:ALA:CB	2.03	0.88
2:B:176:THR:HG23	2:B:178:ASN:H	1.38	0.88
1:A:158:ARG:HH11	2:B:170:ARG:CZ	1.87	0.87
2:B:84:LEU:HD11	2:B:89:CYS:SG	2.17	0.84
2:B:126:GLN:HA	2:B:126:GLN:HE21	1.41	0.84
2:B:114:LEU:HD12	2:B:115:VAL:N	1.94	0.81
1:A:131:GLY:O	1:A:132:THR:HB	1.84	0.78
1:A:95:GLN:HE22	3:A:201:NAG:H62	1.48	0.78
2:B:176:THR:CG2	2:B:179:TRP:H	1.96	0.78
1:A:94:ALA:HA	1:A:168:SER:HB3	1.66	0.77
1:A:114:HIS:CE1	1:A:164:LYS:HE2	2.21	0.76
2:B:114:LEU:HD12	2:B:115:VAL:H	1.50	0.76
1:A:73:SER:O	1:A:164:LYS:HE3	1.87	0.74
2:B:78:CYS:SG	2:B:84:LEU:HD21	2.27	0.74
2:B:142:THR:HG22	2:B:147:LEU:N	2.01	0.73
1:A:114:HIS:HA	1:A:164:LYS:O	1.89	0.73
2:B:169:ASP:O	2:B:170:ARG:HB3	1.89	0.73
1:A:94:ALA:HA	1:A:168:SER:CB	2.18	0.72
1:A:98:THR:HG22	1:A:101:ASP:OD2	1.90	0.71
2:B:114:LEU:HB3	2:B:137:ILE:HG22	1.71	0.71
1:A:115:TRP:H	1:A:165:TRP:HA	1.56	0.70
1:A:116:ILE:HD11	1:A:147:ALA:CB	2.21	0.70
1:A:120:ARG:HD3	1:A:126:TRP:CE2	2.26	0.70
1:A:128:TRP:HE3	1:A:132:THR:HG23	1.56	0.69
1:A:141:ILE:HD11	2:B:188:THR:HG21	1.75	0.69
2:B:98:THR:OG1	2:B:101:GLU:HG3	1.93	0.69
1:A:162:ASP:OD1	2:B:176:THR:HG21	1.93	0.68
2:B:156:LEU:HD22	2:B:157:VAL:H	1.58	0.68
1:A:121:LYS:O	1:A:124:ASP:HB2	1.94	0.68
1:A:110:GLY:CA	1:A:151:ALA:HB2	2.20	0.67
2:B:83:LEU:C	2:B:84:LEU:HD22	2.14	0.67
2:B:176:THR:HG22	2:B:179:TRP:O	1.95	0.66
1:A:161:ILE:HA	2:B:181:TYR:CD2	2.29	0.66
2:B:139:LEU:HG	2:B:150:TRP:NE1	2.10	0.66
1:A:106:LYS:HD2	1:A:151:ALA:O	1.94	0.66
2:B:108:GLN:O	2:B:109:LEU:HD13	1.95	0.66
2:B:143:PHE:HA	2:B:169:ASP:HB3	1.79	0.65
2:B:176:THR:HG22	2:B:179:TRP:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:THR:CG2	2:B:146:ASN:H	2.10	0.65
2:B:141:VAL:HA	2:B:147:LEU:O	1.97	0.65
2:B:136:TRP:O	2:B:137:ILE:HG23	1.96	0.65
2:B:124:PHE:O	2:B:128:SER:HB2	1.97	0.65
1:A:86:CYS:SG	1:A:93:LEU:HD23	2.36	0.64
2:B:142:THR:O	2:B:143:PHE:HB3	1.96	0.64
1:A:95:GLN:NE2	3:A:201:NAG:H62	2.12	0.64
2:B:126:GLN:NE2	2:B:126:GLN:HA	2.12	0.64
2:B:142:THR:HG23	2:B:146:ASN:H	1.62	0.64
1:A:158:ARG:NH1	2:B:170:ARG:CZ	2.60	0.63
2:B:85:ASN:HB2	2:B:124:PHE:CE2	2.32	0.63
1:A:148:PHE:CE1	1:A:155:HIS:HB2	2.35	0.62
2:B:115:VAL:HG12	2:B:194:GLN:NE2	2.15	0.62
2:B:84:LEU:CD1	2:B:89:CYS:HA	2.29	0.62
1:A:70:PHE:HA	1:A:167:CYS:O	1.99	0.61
2:B:156:LEU:HD22	2:B:157:VAL:N	2.15	0.61
1:A:140:ILE:HG22	1:A:140:ILE:O	2.01	0.61
2:B:122:LEU:O	2:B:126:GLN:HB2	1.99	0.61
2:B:188:THR:O	2:B:189:PHE:CD2	2.54	0.61
2:B:84:LEU:HD13	2:B:89:CYS:HA	1.82	0.60
2:B:142:THR:CG2	2:B:147:LEU:H	2.07	0.60
2:B:91:TRP:CZ3	2:B:93:SER:HA	2.37	0.60
2:B:176:THR:HG23	2:B:178:ASN:N	2.13	0.59
1:A:131:GLY:O	1:A:132:THR:CB	2.50	0.59
2:B:101:GLU:O	2:B:104:ARG:HB3	2.02	0.59
1:A:115:TRP:CH2	1:A:159:GLY:HA2	2.38	0.59
1:A:141:ILE:HG13	1:A:142:GLY:N	2.18	0.59
2:B:85:ASN:HB2	2:B:124:PHE:CZ	2.38	0.59
1:A:116:ILE:HD13	1:A:118:LEU:HB2	1.83	0.58
3:A:204:NAG:O3	3:A:205:NAG:H82	2.03	0.58
1:A:128:TRP:HE3	1:A:132:THR:CG2	2.16	0.58
1:A:161:ILE:HD13	2:B:134:PHE:HE1	1.68	0.58
2:B:115:VAL:HG13	2:B:115:VAL:O	2.02	0.58
2:B:130:LYS:HD3	2:B:131:PRO:HD2	1.85	0.58
1:A:120:ARG:HG2	1:A:145:SER:HA	1.86	0.58
2:B:142:THR:CG2	2:B:146:ASN:N	2.67	0.57
1:A:98:THR:HG23	1:A:101:ASP:H	1.70	0.56
2:B:138:GLY:O	2:B:150:TRP:HA	2.05	0.56
2:B:83:LEU:O	2:B:84:LEU:HD22	2.06	0.56
2:B:82:TRP:O	2:B:84:LEU:HD22	2.05	0.56
1:A:129:THR:O	1:A:130:ASN:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ALA:H	1:A:167:CYS:HA	1.71	0.55
2:B:141:VAL:HG12	2:B:142:THR:N	2.21	0.55
2:B:78:CYS:SG	2:B:84:LEU:HD11	2.47	0.55
1:A:141:ILE:O	1:A:155:HIS:HA	2.07	0.55
1:A:87:SER:C	1:A:89:GLN:H	2.09	0.55
1:A:106:LYS:HB3	1:A:151:ALA:HA	1.89	0.55
2:B:156:LEU:C	2:B:156:LEU:HD13	2.27	0.54
2:B:98:THR:O	2:B:101:GLU:HB2	2.07	0.54
1:A:107:ARG:HG2	1:A:107:ARG:HH11	1.71	0.54
1:A:116:ILE:CD1	1:A:118:LEU:HB2	2.37	0.54
2:B:108:GLN:HA	2:B:108:GLN:NE2	2.22	0.53
2:B:170:ARG:HG2	2:B:170:ARG:O	2.07	0.53
1:A:114:HIS:HE1	1:A:164:LYS:HE2	1.69	0.53
1:A:97:ASP:N	1:A:97:ASP:OD2	2.41	0.53
2:B:108:GLN:HA	2:B:108:GLN:HE21	1.73	0.53
2:B:99:TRP:HD1	2:B:136:TRP:CE3	2.26	0.53
2:B:136:TRP:NE1	2:B:189:PHE:HB2	2.24	0.53
2:B:153:GLU:HA	2:B:153:GLU:OE1	2.09	0.52
1:A:141:ILE:CG1	1:A:142:GLY:N	2.73	0.52
2:B:140:TYR:H	2:B:140:TYR:HD2	1.55	0.52
2:B:96:PHE:O	2:B:97:LYS:HG3	2.10	0.52
2:B:141:VAL:CG1	2:B:142:THR:N	2.72	0.52
1:A:122:GLN:O	1:A:124:ASP:N	2.43	0.51
1:A:114:HIS:CE1	1:A:164:LYS:CE	2.93	0.51
2:B:115:VAL:HG12	2:B:194:GLN:HE21	1.75	0.51
1:A:158:ARG:HH11	2:B:170:ARG:NH2	2.07	0.51
2:B:82:TRP:CZ2	2:B:91:TRP:HB2	2.46	0.51
1:A:169:LYS:O	1:A:169:LYS:HG3	2.10	0.50
2:B:148:TRP:HE1	2:B:167:THR:HG22	1.75	0.50
2:B:194:GLN:O	2:B:195:ARG:HB3	2.10	0.50
2:B:115:VAL:CG1	2:B:194:GLN:NE2	2.75	0.50
1:A:84:ILE:HG22	1:A:88:LEU:HD13	1.93	0.50
1:A:141:ILE:HD11	2:B:188:THR:CG2	2.40	0.50
1:A:71:TYR:O	1:A:166:ILE:HA	2.11	0.50
1:A:76:THR:HB	1:A:162:ASP:C	2.33	0.50
1:A:115:TRP:N	1:A:165:TRP:HA	2.24	0.49
1:A:122:GLN:C	1:A:124:ASP:H	2.16	0.49
1:A:138:PHE:HE1	1:A:140:ILE:HD11	1.77	0.49
3:A:201:NAG:H61	3:A:202:NAG:C1	2.43	0.48
2:B:122:LEU:C	2:B:124:PHE:H	2.16	0.48
1:A:73:SER:HB3	1:A:165:TRP:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:LEU:HG	2:B:150:TRP:CD1	2.49	0.48
2:B:149:MET:HB3	2:B:149:MET:HE3	1.74	0.48
1:A:71:TYR:HB3	1:A:167:CYS:HB2	1.96	0.47
1:A:84:ILE:O	1:A:87:SER:HB2	2.14	0.47
1:A:89:GLN:C	1:A:90:LYS:HD3	2.35	0.47
2:B:98:THR:HA	2:B:187:SER:O	2.15	0.47
2:B:134:PHE:C	2:B:134:PHE:CD2	2.87	0.47
1:A:114:HIS:HE1	1:A:164:LYS:CE	2.27	0.47
2:B:90:TYR:HE2	2:B:194:GLN:OE1	1.97	0.47
1:A:114:HIS:HB3	1:A:166:ILE:HG13	1.96	0.47
2:B:169:ASP:O	2:B:170:ARG:CB	2.62	0.47
2:B:107:THR:C	2:B:109:LEU:H	2.18	0.47
2:B:140:TYR:N	2:B:140:TYR:HD2	2.13	0.47
2:B:191:GLY:O	2:B:192:ILE:HD13	2.15	0.47
1:A:95:GLN:NE2	3:A:201:NAG:O6	2.38	0.46
1:A:130:ASN:CG	1:A:131:GLY:H	2.18	0.46
1:A:80:THR:O	1:A:84:ILE:HG13	2.15	0.46
2:B:82:TRP:CE2	2:B:91:TRP:HB2	2.51	0.46
1:A:66:ARG:HB3	1:A:67:ASP:H	1.49	0.46
2:B:140:TYR:N	2:B:140:TYR:CD2	2.83	0.46
2:B:83:LEU:O	2:B:84:LEU:HD13	2.15	0.46
1:A:141:ILE:HD11	2:B:188:THR:OG1	2.16	0.46
2:B:96:PHE:HD2	2:B:189:PHE:HA	1.81	0.46
1:A:128:TRP:CE3	1:A:132:THR:HG23	2.45	0.45
2:B:188:THR:O	2:B:189:PHE:HD2	1.98	0.45
2:B:83:LEU:HD22	2:B:83:LEU:H	1.81	0.45
2:B:109:LEU:O	2:B:110:GLN:C	2.54	0.45
2:B:149:MET:HG2	2:B:150:TRP:N	2.31	0.45
2:B:112:HIS:HD2	2:B:113:LEU:O	1.98	0.45
2:B:114:LEU:O	2:B:138:GLY:N	2.38	0.45
2:B:163:VAL:HA	2:B:180:VAL:O	2.16	0.45
2:B:136:TRP:HZ2	2:B:187:SER:O	1.99	0.45
1:A:120:ARG:HD3	1:A:126:TRP:CZ2	2.51	0.45
2:B:156:LEU:HD13	2:B:157:VAL:N	2.32	0.45
1:A:135:ASN:OD1	1:A:137:TRP:HD1	2.00	0.45
2:B:118:ASN:O	2:B:120:ASP:N	2.50	0.44
1:A:73:SER:OG	1:A:75:ASP:O	2.36	0.44
3:A:204:NAG:H3	3:A:205:NAG:N2	2.33	0.44
2:B:139:LEU:HD22	2:B:148:TRP:HB3	2.00	0.44
2:B:96:PHE:HA	2:B:189:PHE:O	2.16	0.44
1:A:93:LEU:O	1:A:94:ALA:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:SER:OG	2:B:94:THR:N	2.50	0.44
1:A:144:GLY:CA	1:A:156:SER:HB3	2.48	0.44
1:A:109:ALA:O	1:A:110:GLY:C	2.56	0.43
1:A:110:GLY:O	1:A:112:ASP:N	2.52	0.43
1:A:130:ASN:CG	1:A:131:GLY:N	2.72	0.43
2:B:126:GLN:HG3	2:B:177:GLY:O	2.18	0.43
2:B:96:PHE:HB3	2:B:188:THR:HB	2.01	0.43
1:A:162:ASP:OD1	2:B:176:THR:CG2	2.65	0.43
2:B:160:LEU:HD12	2:B:161:PHE:CE2	2.54	0.43
2:B:195:ARG:C	2:B:195:ARG:HD3	2.40	0.42
2:B:86:GLU:O	2:B:88:LYS:N	2.53	0.42
1:A:93:LEU:HB2	1:A:117:GLY:CA	2.50	0.42
2:B:140:TYR:CD2	2:B:149:MET:O	2.73	0.42
1:A:161:ILE:HD12	1:A:163:ILE:HG21	2.02	0.42
2:B:142:THR:O	2:B:143:PHE:CB	2.65	0.41
2:B:83:LEU:N	2:B:83:LEU:HD22	2.35	0.41
2:B:144:GLN:HG3	2:B:145:GLY:N	2.36	0.41
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.84	0.41
1:A:114:HIS:O	1:A:148:PHE:HA	2.21	0.41
1:A:93:LEU:HB3	1:A:117:GLY:N	2.35	0.41
1:A:158:ARG:NH1	2:B:170:ARG:NH1	2.69	0.41
1:A:114:HIS:HE1	1:A:164:LYS:NZ	2.19	0.41
1:A:161:ILE:HG22	2:B:181:TYR:CD2	2.56	0.40
1:A:93:LEU:HD12	1:A:117:GLY:HA2	2.02	0.40
2:B:111:ALA:HB2	2:B:195:ARG:HG2	2.04	0.40
2:B:130:LYS:HA	2:B:131:PRO:HD2	1.78	0.40
1:A:104:PHE:CD2	1:A:105:LEU:HD23	2.57	0.40
2:B:92:PHE:CD1	2:B:192:ILE:HD12	2.56	0.40
2:B:82:TRP:CE3	2:B:89:CYS:HB3	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	115/142 (81%)	82 (71%)	17 (15%)	16 (14%)	0	1
2	B	119/158 (75%)	78 (66%)	29 (24%)	12 (10%)	1	4
All	All	234/300 (78%)	160 (68%)	46 (20%)	28 (12%)	0	2

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ALA
1	A	124	ASP
1	A	130	ASN
1	A	132	THR
1	A	135	ASN
2	B	79	PRO
2	B	119	LEU
1	A	93	LEU
1	A	110	GLY
1	A	111	THR
1	A	122	GLN
1	A	128	TRP
2	B	87	GLY
2	B	93	SER
1	A	59	SER
1	A	123	GLY
1	A	136	GLY
1	A	143	ASN
2	B	94	THR
2	B	195	ARG
2	B	116	ILE
2	B	131	PRO
2	B	144	GLN
1	A	109	ALA
2	B	83	LEU
2	B	138	GLY
2	B	192	ILE
1	A	140	ILE

### 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	93/118 (79%)	84 (90%)	9 (10%)	9	36
2	B	101/140 (72%)	86 (85%)	15 (15%)	3	16
All	All	194/258 (75%)	170 (88%)	24 (12%)	5	24

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	89	GLN
1	A	90	LYS
1	A	95	GLN
1	A	97	ASP
1	A	113	MET
1	A	129	THR
1	A	141	ILE
1	A	154	VAL
2	B	78	CYS
2	B	86	GLU
2	B	98	THR
2	B	108	GLN
2	B	110	GLN
2	B	121	GLU
2	B	126	GLN
2	B	134	PHE
2	B	140	TYR
2	B	149	MET
2	B	156	LEU
2	B	160	LEU
2	B	170	ARG
2	B	195	ARG
2	B	196	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	95	GLN
1	A	114	HIS

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Mol	Chain	Res	Type
2	B	108	GLN
2	B	110	GLN
2	B	112	HIS
2	B	126	GLN
2	B	127	ASN
2	B	194	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	A	201	1,3	14,14,15	0.82	0	15,19,21	0.94	1 (6%)
3	NAG	A	202	3,4	14,14,15	0.76	0	15,19,21	0.85	0
4	MAN	A	203	3	11,11,12	0.87	0	13,15,17	0.93	1 (7%)
3	NAG	A	204	1,3	14,14,15	0.93	0	15,19,21	1.80	4 (26%)
3	NAG	A	205	3,4	14,14,15	1.43	3 (21%)	15,19,21	1.90	3 (20%)
4	MAN	A	206	3	11,11,12	0.59	0	13,15,17	1.51	1 (7%)



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	201	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	202	3,4	-	0/6/23/26	0/1/1/1
4	MAN	A	203	3	-	0/2/19/22	0/1/1/1
3	NAG	A	204	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	205	3,4	-	0/6/23/26	0/1/1/1
4	MAN	A	206	3	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	205	NAG	O5-C1	2.39	1.47	1.43
3	A	205	NAG	O5-C5	2.71	1.49	1.43
3	A	205	NAG	C1-C2	3.22	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	204	NAG	C4-C3-C2	-4.14	104.95	111.02
3	A	205	NAG	C4-C3-C2	-3.44	105.97	111.02
3	A	204	NAG	C3-C4-C5	-3.35	104.31	110.22
3	A	201	NAG	C2-N2-C7	-2.14	119.82	122.94
3	A	204	NAG	O4-C4-C5	2.17	114.76	109.28
4	A	203	MAN	C1-C2-C3	2.68	113.04	109.65
3	A	204	NAG	C1-O5-C5	2.82	116.06	112.17
3	A	205	NAG	O5-C1-C2	3.59	116.46	111.47
4	A	206	MAN	C1-C2-C3	4.47	115.32	109.65
3	A	205	NAG	C1-O5-C5	4.70	118.64	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	NAG	5	0
3	A	202	NAG	1	0
3	A	204	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	205	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	117/142 (82%)	0.10	5 (4%) 36 23	41, 96, 153, 179	0
2	B	121/158 (76%)	0.08	1 (0%) 86 77	44, 98, 133, 176	0
All	All	238/300 (79%)	0.09	6 (2%) 58 43	41, 97, 145, 179	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	ILE	2.6
1	A	159	GLY	2.5
1	A	96	ILE	2.5
1	A	128	TRP	2.2
1	A	118	LEU	2.1
2	B	174	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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	204	14/15	0.85	0.18	-0.83	103,103,103,103	0
3	NAG	A	201	14/15	0.91	0.16	-1.24	158,158,158,158	0
4	MAN	A	206	11/12	0.85	0.19	-	138,138,138,138	0
3	NAG	A	205	14/15	0.86	0.27	-	178,178,178,178	0
3	NAG	A	202	14/15	0.88	0.20	-	123,123,123,123	0
4	MAN	A	203	11/12	0.76	0.23	-	146,146,146,146	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.