



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 02:16 PM BST

PDB ID : 6E7D  
Title : Structure of the inhibitory NKRP1B receptor bound to the host-encoded ligand, Clr-b  
Authors : Balaji, G.R.; Rossjohn, J.; Berry, R.  
Deposited on : 2018-07-26  
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (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

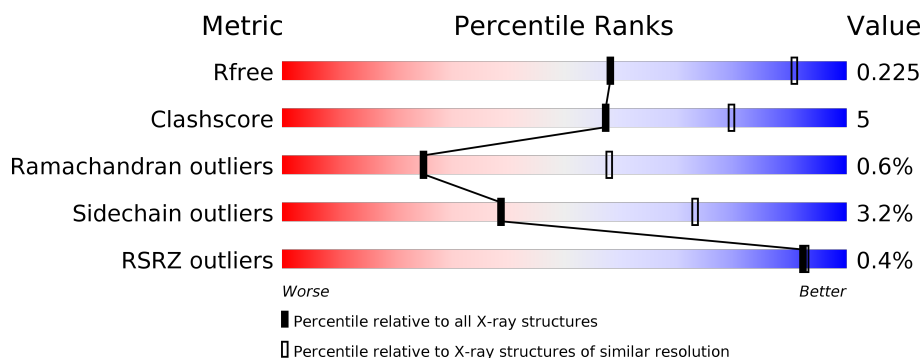
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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.




















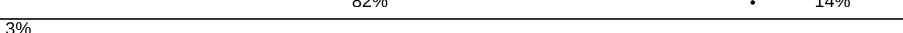
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	124	<div> <div>77%</div> <div>20%</div> <div>..</div> </div>
1	B	124	<div> <div>%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	C	124	<div> <div>85%</div> <div>10%</div> <div>..</div> </div>
1	D	124	<div> <div>82%</div> <div>13%</div> <div>..</div> </div>
1	E	124	<div> <div>80%</div> <div>18%</div> <div>..</div> </div>
1	F	124	<div> <div>79%</div> <div>19%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	124	
1	H	124	
1	I	124	
1	J	124	
1	K	124	
1	L	124	
1	M	124	
1	N	124	
1	O	124	
1	P	124	
2	Q	137	
2	R	137	
2	S	137	
2	T	137	
2	U	137	
2	V	137	
2	W	137	
2	X	137	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22989 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 D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			997	635	171	184	7			
1	B	121	Total	C	N	O	S	0	0	0
			974	624	169	173	8			
1	C	120	Total	C	N	O	S	0	0	0
			979	625	166	181	7			
1	D	121	Total	C	N	O	S	0	0	0
			1006	641	173	185	7			
1	E	122	Total	C	N	O	S	0	0	0
			994	637	175	175	7			
1	F	122	Total	C	N	O	S	0	0	0
			982	629	170	176	7			
1	G	119	Total	C	N	O	S	0	0	0
			986	630	170	179	7			
1	H	122	Total	C	N	O	S	0	0	0
			984	632	168	177	7			
1	I	119	Total	C	N	O	S	0	0	0
			993	634	171	181	7			
1	J	122	Total	C	N	O	S	0	0	0
			987	634	170	175	8			
1	K	118	Total	C	N	O	S	0	0	0
			984	625	171	181	7			
1	L	122	Total	C	N	O	S	0	0	0
			993	639	172	174	8			
1	M	119	Total	C	N	O	S	0	0	0
			983	628	170	178	7			
1	N	122	Total	C	N	O	S	0	0	0
			979	628	170	174	7			
1	O	118	Total	C	N	O	S	0	0	0
			960	615	167	171	7			
1	P	122	Total	C	N	O	S	0	0	0
			1002	639	175	181	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	MET	-	initiating methionine	UNP Q91V08
A	195	ALA	-	expression tag	UNP Q91V08
A	196	SER	-	expression tag	UNP Q91V08
B	73	MET	-	initiating methionine	UNP Q91V08
B	195	ALA	-	expression tag	UNP Q91V08
B	196	SER	-	expression tag	UNP Q91V08
C	73	MET	-	initiating methionine	UNP Q91V08
C	195	ALA	-	expression tag	UNP Q91V08
C	196	SER	-	expression tag	UNP Q91V08
D	73	MET	-	initiating methionine	UNP Q91V08
D	195	ALA	-	expression tag	UNP Q91V08
D	196	SER	-	expression tag	UNP Q91V08
E	73	MET	-	initiating methionine	UNP Q91V08
E	195	ALA	-	expression tag	UNP Q91V08
E	196	SER	-	expression tag	UNP Q91V08
F	73	MET	-	initiating methionine	UNP Q91V08
F	195	ALA	-	expression tag	UNP Q91V08
F	196	SER	-	expression tag	UNP Q91V08
G	73	MET	-	initiating methionine	UNP Q91V08
G	195	ALA	-	expression tag	UNP Q91V08
G	196	SER	-	expression tag	UNP Q91V08
H	73	MET	-	initiating methionine	UNP Q91V08
H	195	ALA	-	expression tag	UNP Q91V08
H	196	SER	-	expression tag	UNP Q91V08
I	73	MET	-	initiating methionine	UNP Q91V08
I	195	ALA	-	expression tag	UNP Q91V08
I	196	SER	-	expression tag	UNP Q91V08
J	73	MET	-	initiating methionine	UNP Q91V08
J	195	ALA	-	expression tag	UNP Q91V08
J	196	SER	-	expression tag	UNP Q91V08
K	73	MET	-	initiating methionine	UNP Q91V08
K	195	ALA	-	expression tag	UNP Q91V08
K	196	SER	-	expression tag	UNP Q91V08
L	73	MET	-	initiating methionine	UNP Q91V08
L	195	ALA	-	expression tag	UNP Q91V08
L	196	SER	-	expression tag	UNP Q91V08
M	73	MET	-	initiating methionine	UNP Q91V08
M	195	ALA	-	expression tag	UNP Q91V08
M	196	SER	-	expression tag	UNP Q91V08
N	73	MET	-	initiating methionine	UNP Q91V08
N	195	ALA	-	expression tag	UNP Q91V08
N	196	SER	-	expression tag	UNP Q91V08

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Chain	Residue	Modelled	Actual	Comment	Reference
O	73	MET	-	initiating methionine	UNP Q91V08
O	195	ALA	-	expression tag	UNP Q91V08
O	196	SER	-	expression tag	UNP Q91V08
P	73	MET	-	initiating methionine	UNP Q91V08
P	195	ALA	-	expression tag	UNP Q91V08
P	196	SER	-	expression tag	UNP Q91V08

- Molecule 2 is a protein called Killer cell lectin-like receptor subfamily B member 1B allele B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	117	Total	C	N	O	S	0	0	0
			892	561	152	173	6			
2	R	112	Total	C	N	O	S	0	0	0
			812	514	136	157	5			
2	S	122	Total	C	N	O	S	0	0	0
			918	573	154	184	7			
2	T	122	Total	C	N	O	S	0	0	0
			924	579	155	183	7			
2	U	116	Total	C	N	O	S	0	0	0
			861	541	149	164	7			
2	V	121	Total	C	N	O	S	0	0	0
			897	564	151	175	7			
2	W	118	Total	C	N	O	S	0	0	0
			876	546	149	174	7			
2	X	119	Total	C	N	O	S	0	0	0
			861	538	144	172	7			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	87	THR	-	expression tag	UNP Q99JB4
Q	88	GLY	-	expression tag	UNP Q99JB4
Q	118	GLY	CYS	engineered mutation	UNP Q99JB4
Q	216	GLY	-	expression tag	UNP Q99JB4
Q	217	THR	-	expression tag	UNP Q99JB4
Q	218	HIS	-	expression tag	UNP Q99JB4
Q	219	HIS	-	expression tag	UNP Q99JB4
Q	220	HIS	-	expression tag	UNP Q99JB4
Q	221	HIS	-	expression tag	UNP Q99JB4
Q	222	HIS	-	expression tag	UNP Q99JB4
Q	223	HIS	-	expression tag	UNP Q99JB4
R	87	THR	-	expression tag	UNP Q99JB4

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Chain	Residue	Modelled	Actual	Comment	Reference
R	88	GLY	-	expression tag	UNP Q99JB4
R	118	GLY	CYS	engineered mutation	UNP Q99JB4
R	216	GLY	-	expression tag	UNP Q99JB4
R	217	THR	-	expression tag	UNP Q99JB4
R	218	HIS	-	expression tag	UNP Q99JB4
R	219	HIS	-	expression tag	UNP Q99JB4
R	220	HIS	-	expression tag	UNP Q99JB4
R	221	HIS	-	expression tag	UNP Q99JB4
R	222	HIS	-	expression tag	UNP Q99JB4
R	223	HIS	-	expression tag	UNP Q99JB4
S	87	THR	-	expression tag	UNP Q99JB4
S	88	GLY	-	expression tag	UNP Q99JB4
S	118	GLY	CYS	engineered mutation	UNP Q99JB4
S	216	GLY	-	expression tag	UNP Q99JB4
S	217	THR	-	expression tag	UNP Q99JB4
S	218	HIS	-	expression tag	UNP Q99JB4
S	219	HIS	-	expression tag	UNP Q99JB4
S	220	HIS	-	expression tag	UNP Q99JB4
S	221	HIS	-	expression tag	UNP Q99JB4
S	222	HIS	-	expression tag	UNP Q99JB4
S	223	HIS	-	expression tag	UNP Q99JB4
T	87	THR	-	expression tag	UNP Q99JB4
T	88	GLY	-	expression tag	UNP Q99JB4
T	118	GLY	CYS	engineered mutation	UNP Q99JB4
T	216	GLY	-	expression tag	UNP Q99JB4
T	217	THR	-	expression tag	UNP Q99JB4
T	218	HIS	-	expression tag	UNP Q99JB4
T	219	HIS	-	expression tag	UNP Q99JB4
T	220	HIS	-	expression tag	UNP Q99JB4
T	221	HIS	-	expression tag	UNP Q99JB4
T	222	HIS	-	expression tag	UNP Q99JB4
T	223	HIS	-	expression tag	UNP Q99JB4
U	87	THR	-	expression tag	UNP Q99JB4
U	88	GLY	-	expression tag	UNP Q99JB4
U	118	GLY	CYS	engineered mutation	UNP Q99JB4
U	216	GLY	-	expression tag	UNP Q99JB4
U	217	THR	-	expression tag	UNP Q99JB4
U	218	HIS	-	expression tag	UNP Q99JB4
U	219	HIS	-	expression tag	UNP Q99JB4
U	220	HIS	-	expression tag	UNP Q99JB4
U	221	HIS	-	expression tag	UNP Q99JB4
U	222	HIS	-	expression tag	UNP Q99JB4

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Chain	Residue	Modelled	Actual	Comment	Reference
U	223	HIS	-	expression tag	UNP Q99JB4
V	87	THR	-	expression tag	UNP Q99JB4
V	88	GLY	-	expression tag	UNP Q99JB4
V	118	GLY	CYS	engineered mutation	UNP Q99JB4
V	216	GLY	-	expression tag	UNP Q99JB4
V	217	THR	-	expression tag	UNP Q99JB4
V	218	HIS	-	expression tag	UNP Q99JB4
V	219	HIS	-	expression tag	UNP Q99JB4
V	220	HIS	-	expression tag	UNP Q99JB4
V	221	HIS	-	expression tag	UNP Q99JB4
V	222	HIS	-	expression tag	UNP Q99JB4
V	223	HIS	-	expression tag	UNP Q99JB4
W	87	THR	-	expression tag	UNP Q99JB4
W	88	GLY	-	expression tag	UNP Q99JB4
W	118	GLY	CYS	engineered mutation	UNP Q99JB4
W	216	GLY	-	expression tag	UNP Q99JB4
W	217	THR	-	expression tag	UNP Q99JB4
W	218	HIS	-	expression tag	UNP Q99JB4
W	219	HIS	-	expression tag	UNP Q99JB4
W	220	HIS	-	expression tag	UNP Q99JB4
W	221	HIS	-	expression tag	UNP Q99JB4
W	222	HIS	-	expression tag	UNP Q99JB4
W	223	HIS	-	expression tag	UNP Q99JB4
X	87	THR	-	expression tag	UNP Q99JB4
X	88	GLY	-	expression tag	UNP Q99JB4
X	118	GLY	CYS	engineered mutation	UNP Q99JB4
X	216	GLY	-	expression tag	UNP Q99JB4
X	217	THR	-	expression tag	UNP Q99JB4
X	218	HIS	-	expression tag	UNP Q99JB4
X	219	HIS	-	expression tag	UNP Q99JB4
X	220	HIS	-	expression tag	UNP Q99JB4
X	221	HIS	-	expression tag	UNP Q99JB4
X	222	HIS	-	expression tag	UNP Q99JB4
X	223	HIS	-	expression tag	UNP Q99JB4

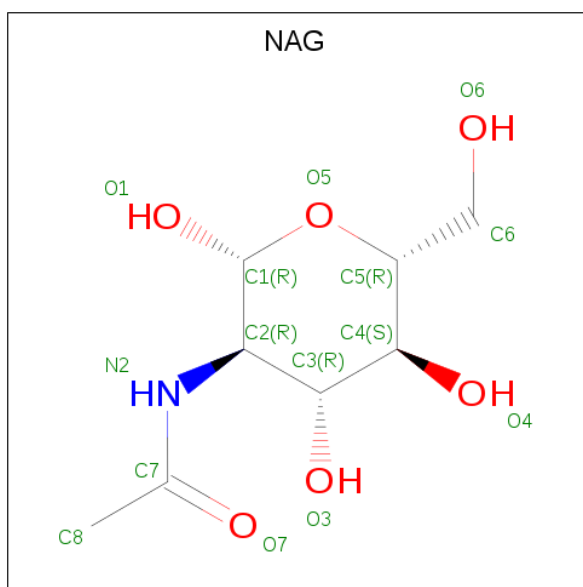
- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		
3	S	1	Total	O	S	0	0
			5	4	1		
3	T	1	Total	O	S	0	0
			5	4	1		
3	U	1	Total	O	S	0	0
			5	4	1		
3	V	1	Total	O	S	0	0
			5	4	1		
3	W	1	Total	O	S	0	0
			5	4	1		
3	X	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	Q	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		
4	S	1	Total	C	N	O	0	0
			14	8	1	5		
4	T	1	Total	C	N	O	0	0
			14	8	1	5		
4	U	1	Total	C	N	O	0	0
			14	8	1	5		
4	V	1	Total	C	N	O	0	0
			14	8	1	5		
4	W	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	O	0	0
			2	2		
5	F	1	Total	O	0	0
			1	1		
5	H	1	Total	O	0	0
			1	1		
5	K	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	O	0	0
			1	1		
5	O	1	Total	O	0	0
			1	1		

### 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.

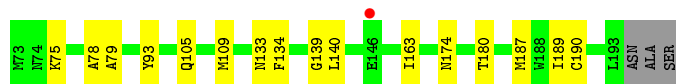
- Molecule 1: C-type lectin domain family 2 member D

Chain A: 




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

Chain B: 




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

Chain C: 




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

Chain D: 



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

Chain E: 

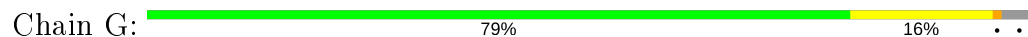


- Molecule 1: C-type lectin domain family 2 member D

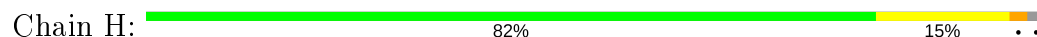
Chain F: 



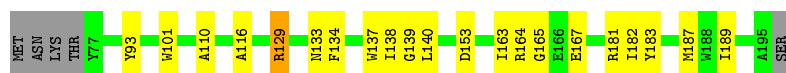
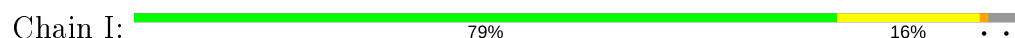
- Molecule 1: C-type lectin domain family 2 member D



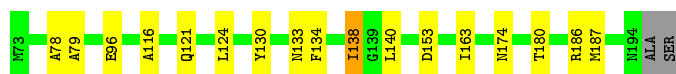
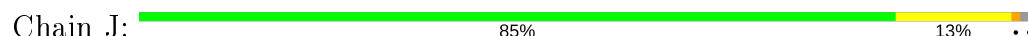
- Molecule 1: C-type lectin domain family 2 member D



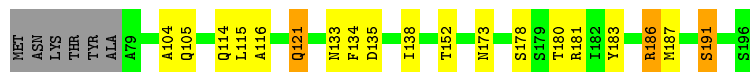
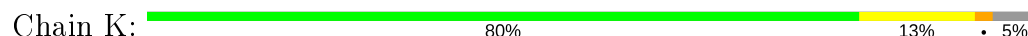
- Molecule 1: C-type lectin domain family 2 member D



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



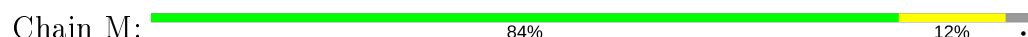
- Molecule 1: C-type lectin domain family 2 member D



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

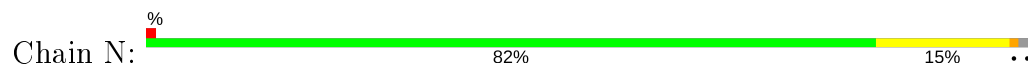


- Molecule 1: C-type lectin domain family 2 member D

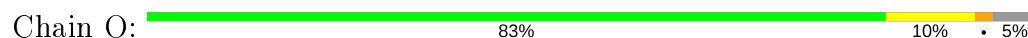




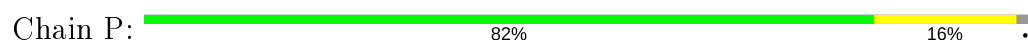
- Molecule 1: C-type lectin domain family 2 member D



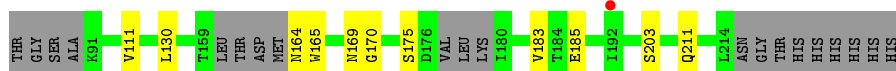
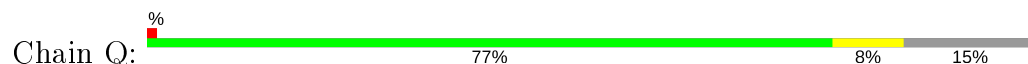
- Molecule 1: C-type lectin domain family 2 member D



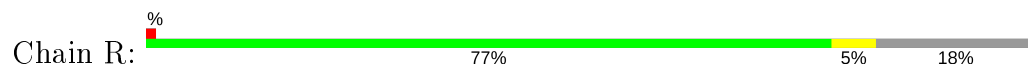
- Molecule 1: C-type lectin domain family 2 member D



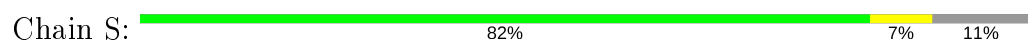
- Molecule 2: Killer cell lectin-like receptor subfamily B member 1B allele B



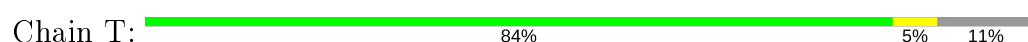
- Molecule 2: Killer cell lectin-like receptor subfamily B member 1B allele B

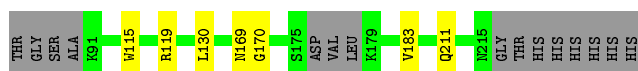


- Molecule 2: Killer cell lectin-like receptor subfamily B member 1B allele B

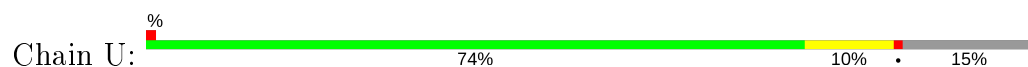


- Molecule 2: Killer cell lectin-like receptor subfamily B member 1B allele B

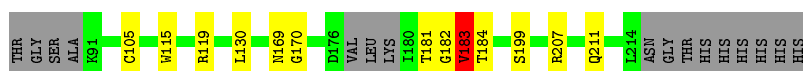




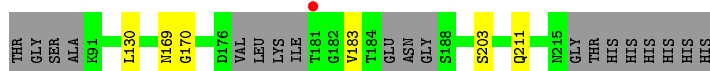
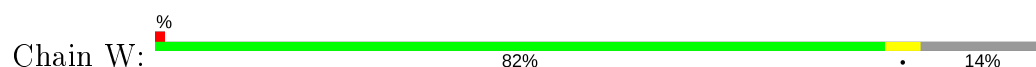
- Molecule 2: Killer cell lectin-like receptor subfamily B member 1B allele B



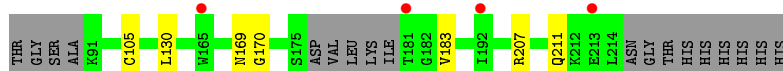
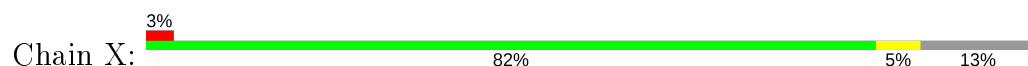
- Molecule 2: Killer cell lectin-like receptor subfamily B member 1B allele B



- Molecule 2: Killer cell lectin-like receptor subfamily B member 1B allele B



- Molecule 2: Killer cell lectin-like receptor subfamily B member 1B allele B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.93Å 122.07Å 131.56Å 73.12° 82.08° 84.46°	Depositor
Resolution (Å)	42.46 – 2.90 66.17 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.6 (42.46-2.90) 92.5 (66.17-2.90)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.186 , 0.225 0.206 , 0.225	Depositor DCC
$R_{free}$ test set	4054 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	22989	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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, SO4

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	0.55	0/1029	0.72	0/1399
1	B	0.50	0/1006	0.70	0/1370
1	C	0.52	0/1011	0.71	0/1377
1	D	0.59	0/1038	0.76	0/1410
1	E	0.52	0/1026	0.71	0/1396
1	F	0.55	0/1014	0.70	0/1381
1	G	0.56	0/1018	0.75	0/1384
1	H	0.55	0/1016	0.72	0/1385
1	I	0.58	0/1025	0.77	0/1392
1	J	0.53	0/1019	0.69	0/1387
1	K	0.58	0/1015	0.78	0/1377
1	L	0.53	0/1025	0.70	0/1393
1	M	0.50	0/1015	0.71	0/1379
1	N	0.49	0/1011	0.67	0/1378
1	O	0.53	0/990	0.73	0/1345
1	P	0.54	0/1034	0.69	0/1406
2	Q	0.49	0/910	0.71	0/1235
2	R	0.45	0/829	0.68	0/1128
2	S	0.50	0/937	0.69	0/1276
2	T	0.48	0/943	0.70	0/1282
2	U	0.51	0/880	0.72	0/1197
2	V	0.56	0/916	0.75	0/1248
2	W	0.46	0/894	0.66	0/1216
2	X	0.48	0/880	0.69	0/1202
All	All	0.53	0/23481	0.71	0/31943

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	997	0	899	21	0
1	B	974	0	861	7	0
1	C	979	0	867	9	0
1	D	1006	0	917	10	0
1	E	994	0	898	12	0
1	F	982	0	873	16	0
1	G	986	0	892	11	0
1	H	984	0	873	12	0
1	I	993	0	905	15	0
1	J	987	0	877	8	0
1	K	984	0	895	14	0
1	L	993	0	897	4	0
1	M	983	0	888	12	0
1	N	979	0	855	13	0
1	O	960	0	875	11	0
1	P	1002	0	899	9	0
2	Q	892	0	795	6	0
2	R	812	0	685	3	0
2	S	918	0	800	5	0
2	T	924	0	818	3	0
2	U	861	0	756	26	0
2	V	897	0	786	17	0
2	W	876	0	735	3	0
2	X	861	0	709	4	0
3	D	5	0	0	0	0
3	Q	5	0	0	0	0
3	R	5	0	0	0	0
3	S	5	0	0	0	0
3	T	5	0	0	0	0
3	U	5	0	0	0	0
3	V	5	0	0	0	0
3	W	5	0	0	0	0
3	X	5	0	0	0	0
4	Q	14	0	13	0	0
4	R	14	0	13	0	0
4	S	14	0	13	0	0
4	T	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	U	14	0	13	0	0
4	V	14	0	13	0	0
4	W	14	0	13	0	0
4	X	14	0	13	0	0
5	C	2	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	K	2	0	0	0	0
5	M	1	0	0	0	0
5	O	1	0	0	0	0
All	All	22989	0	20359	211	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 5.

The worst 5 of 211 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:U:183:VAL:HG21	2:U:199:SER:N	1.65	1.11
2:V:183:VAL:HG21	2:V:199:SER:N	1.66	1.11
2:U:183:VAL:HG21	2:U:199:SER:H	0.98	1.09
2:V:183:VAL:HG21	2:V:199:SER:H	1.01	1.08
2:U:183:VAL:CG2	2:U:199:SER:H	1.79	0.95

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	119/124 (96%)	111 (93%)	8 (7%)	0	100	100
1	B	119/124 (96%)	110 (92%)	8 (7%)	1 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	118/124 (95%)	109 (92%)	9 (8%)	0	100	100
1	D	119/124 (96%)	113 (95%)	6 (5%)	0	100	100
1	E	120/124 (97%)	111 (92%)	8 (7%)	1 (1%)	19	51
1	F	120/124 (97%)	113 (94%)	6 (5%)	1 (1%)	19	51
1	G	117/124 (94%)	110 (94%)	6 (5%)	1 (1%)	17	48
1	H	120/124 (97%)	111 (92%)	8 (7%)	1 (1%)	19	51
1	I	117/124 (94%)	113 (97%)	3 (3%)	1 (1%)	17	48
1	J	120/124 (97%)	110 (92%)	10 (8%)	0	100	100
1	K	116/124 (94%)	111 (96%)	5 (4%)	0	100	100
1	L	120/124 (97%)	111 (92%)	8 (7%)	1 (1%)	19	51
1	M	117/124 (94%)	112 (96%)	5 (4%)	0	100	100
1	N	120/124 (97%)	112 (93%)	7 (6%)	1 (1%)	19	51
1	O	116/124 (94%)	110 (95%)	6 (5%)	0	100	100
1	P	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
2	Q	111/137 (81%)	102 (92%)	8 (7%)	1 (1%)	17	48
2	R	104/137 (76%)	97 (93%)	6 (6%)	1 (1%)	15	45
2	S	118/137 (86%)	108 (92%)	9 (8%)	1 (1%)	19	51
2	T	118/137 (86%)	108 (92%)	9 (8%)	1 (1%)	19	51
2	U	112/137 (82%)	103 (92%)	8 (7%)	1 (1%)	17	48
2	V	117/137 (85%)	105 (90%)	11 (9%)	1 (1%)	17	48
2	W	112/137 (82%)	104 (93%)	7 (6%)	1 (1%)	17	48
2	X	115/137 (84%)	106 (92%)	8 (7%)	1 (1%)	17	48
All	All	2805/3080 (91%)	2613 (93%)	176 (6%)	16 (1%)	25	58

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	116	ALA
2	Q	183	VAL
2	R	183	VAL
2	S	183	VAL
2	T	183	VAL

### 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	103/110 (94%)	100 (97%)	3 (3%)	42	76
1	B	95/110 (86%)	92 (97%)	3 (3%)	39	73
1	C	99/110 (90%)	96 (97%)	3 (3%)	41	75
1	D	105/110 (96%)	99 (94%)	6 (6%)	20	51
1	E	99/110 (90%)	95 (96%)	4 (4%)	31	65
1	F	97/110 (88%)	94 (97%)	3 (3%)	40	74
1	G	101/110 (92%)	95 (94%)	6 (6%)	19	49
1	H	97/110 (88%)	91 (94%)	6 (6%)	18	47
1	I	103/110 (94%)	98 (95%)	5 (5%)	25	57
1	J	96/110 (87%)	92 (96%)	4 (4%)	30	63
1	K	103/110 (94%)	99 (96%)	4 (4%)	32	66
1	L	98/110 (89%)	92 (94%)	6 (6%)	18	48
1	M	100/110 (91%)	99 (99%)	1 (1%)	76	92
1	N	93/110 (84%)	92 (99%)	1 (1%)	73	92
1	O	97/110 (88%)	94 (97%)	3 (3%)	40	74
1	P	101/110 (92%)	94 (93%)	7 (7%)	15	41
2	Q	91/122 (75%)	89 (98%)	2 (2%)	52	81
2	R	76/122 (62%)	75 (99%)	1 (1%)	69	90
2	S	94/122 (77%)	94 (100%)	0	100	100
2	T	95/122 (78%)	95 (100%)	0	100	100
2	U	85/122 (70%)	83 (98%)	2 (2%)	49	79
2	V	90/122 (74%)	88 (98%)	2 (2%)	52	81
2	W	85/122 (70%)	85 (100%)	0	100	100
2	X	81/122 (66%)	81 (100%)	0	100	100
All	All	2284/2736 (84%)	2212 (97%)	72 (3%)	39	73

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	182	ILE
1	J	138	ILE
2	Q	175	SER
1	H	191	SER
1	I	167	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	133	ASN
1	K	133	ASN
1	P	121	GLN
1	J	121	GLN
1	K	173	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

17 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
4	NAG	V	300	2	14,14,15	0.28	0	17,19,21	0.90	1 (5%)
4	NAG	T	300	2	14,14,15	0.33	0	17,19,21	0.72	1 (5%)
3	SO4	X	302	-	4,4,4	0.21	0	6,6,6	0.30	0
4	NAG	X	301	2	14,14,15	0.32	0	17,19,21	0.76	2 (11%)
3	SO4	D	201	-	4,4,4	0.07	0	6,6,6	0.22	0
4	NAG	U	300	2	14,14,15	0.30	0	17,19,21	0.96	2 (11%)
4	NAG	S	300	2	14,14,15	0.28	0	17,19,21	0.82	2 (11%)
4	NAG	W	300	2	14,14,15	0.30	0	17,19,21	0.74	1 (5%)
3	SO4	S	301	-	4,4,4	0.29	0	6,6,6	0.30	0
3	SO4	T	301	-	4,4,4	0.38	0	6,6,6	0.21	0
3	SO4	Q	301	-	4,4,4	0.41	0	6,6,6	0.36	0
3	SO4	R	301	-	4,4,4	0.15	0	6,6,6	0.19	0
3	SO4	W	301	-	4,4,4	0.20	0	6,6,6	0.19	0
4	NAG	Q	300	2	14,14,15	0.32	0	17,19,21	0.84	2 (11%)
3	SO4	U	301	-	4,4,4	0.19	0	6,6,6	0.23	0
3	SO4	V	301	-	4,4,4	0.14	0	6,6,6	0.31	0
4	NAG	R	300	2	14,14,15	0.32	0	17,19,21	0.90	2 (11%)

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	V	300	2	-	0/6/23/26	0/1/1/1
4	NAG	T	300	2	-	0/6/23/26	0/1/1/1
4	NAG	X	301	2	-	0/6/23/26	0/1/1/1
4	NAG	U	300	2	-	0/6/23/26	0/1/1/1
4	NAG	S	300	2	-	0/6/23/26	0/1/1/1
4	NAG	W	300	2	-	0/6/23/26	0/1/1/1
4	NAG	Q	300	2	-	0/6/23/26	0/1/1/1
4	NAG	R	300	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	300	NAG	C1-O5-C5	2.78	115.95	112.19
4	U	300	NAG	C1-O5-C5	2.62	115.74	112.19
4	V	300	NAG	C1-O5-C5	2.61	115.73	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	300	NAG	O5-C1-C2	-2.51	107.33	111.29
4	Q	300	NAG	C1-O5-C5	2.39	115.43	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	121/124 (97%)	-0.31	0 100 100	20, 40, 71, 81	1 (0%)
1	B	121/124 (97%)	-0.18	1 (0%) 86 86	24, 56, 101, 117	1 (0%)
1	C	120/124 (96%)	-0.12	0 100 100	27, 52, 83, 107	1 (0%)
1	D	121/124 (97%)	-0.37	0 100 100	16, 34, 60, 82	1 (0%)
1	E	122/124 (98%)	-0.28	0 100 100	19, 48, 90, 102	0
1	F	122/124 (98%)	-0.41	0 100 100	15, 40, 88, 106	1 (0%)
1	G	119/124 (95%)	-0.37	0 100 100	19, 35, 66, 86	1 (0%)
1	H	122/124 (98%)	-0.35	0 100 100	14, 44, 89, 111	1 (0%)
1	I	119/124 (95%)	-0.31	0 100 100	10, 33, 60, 87	1 (0%)
1	J	122/124 (98%)	-0.21	0 100 100	11, 49, 94, 106	1 (0%)
1	K	118/124 (95%)	-0.35	0 100 100	12, 32, 65, 87	1 (0%)
1	L	122/124 (98%)	-0.23	1 (0%) 86 86	12, 43, 95, 114	1 (0%)
1	M	119/124 (95%)	-0.26	0 100 100	22, 47, 74, 97	1 (0%)
1	N	122/124 (98%)	-0.14	1 (0%) 86 86	23, 52, 96, 114	1 (0%)
1	O	118/124 (95%)	-0.24	0 100 100	28, 49, 77, 94	1 (0%)
1	P	122/124 (98%)	-0.23	0 100 100	18, 45, 81, 96	1 (0%)
2	Q	117/137 (85%)	-0.11	1 (0%) 84 84	29, 62, 85, 100	1 (0%)
2	R	112/137 (81%)	0.26	1 (0%) 84 84	43, 81, 103, 111	0
2	S	122/137 (89%)	-0.02	0 100 100	26, 59, 94, 120	2 (1%)
2	T	122/137 (89%)	-0.21	0 100 100	20, 56, 88, 124	1 (0%)
2	U	116/137 (84%)	-0.18	1 (0%) 84 84	24, 62, 99, 125	0
2	V	121/137 (88%)	-0.31	0 100 100	17, 51, 83, 101	1 (0%)
2	W	118/137 (86%)	-0.11	1 (0%) 86 86	38, 69, 103, 125	2 (1%)
2	X	119/137 (86%)	0.08	4 (3%) 45 40	42, 77, 119, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	2877/3080 (93%)	-0.21	11 (0%) 92 93	10, 51, 95, 144	22 (0%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	95	PRO	2.9
2	X	181	THR	2.3
2	U	140	PHE	2.3
2	W	181	THR	2.3
2	X	165	TRP	2.3

## 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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	X	301	14/15	0.85	0.24	114,125,136,136	0
4	NAG	U	300	14/15	0.87	0.20	80,98,114,119	0
4	NAG	R	300	14/15	0.88	0.24	93,97,108,111	0
4	NAG	S	300	14/15	0.90	0.15	72,86,97,97	0
4	NAG	Q	300	14/15	0.93	0.17	58,68,71,73	0
4	NAG	W	300	14/15	0.93	0.15	79,93,100,101	0
4	NAG	V	300	14/15	0.94	0.17	43,58,75,76	0
3	SO4	D	201	5/5	0.95	0.12	109,109,110,110	0
4	NAG	T	300	14/15	0.95	0.17	46,62,76,78	0
3	SO4	R	301	5/5	0.96	0.10	86,88,89,93	0
3	SO4	U	301	5/5	0.97	0.14	77,78,84,85	0
3	SO4	Q	301	5/5	0.97	0.15	52,57,58,62	0
3	SO4	W	301	5/5	0.99	0.12	62,64,65,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	T	301	5/5	0.99	0.12	50,52,54,56	0
3	SO4	X	302	5/5	0.99	0.11	65,67,67,69	0
3	SO4	V	301	5/5	0.99	0.11	50,51,53,54	0
3	SO4	S	301	5/5	0.99	0.12	62,63,64,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.