



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2025 – 12:39 pm GMT

PDB ID : 8QMD
Title : Human NK cell receptor NKp80, extracellular domain
Authors : Blaha, J.; Pazderova, K.; Kalouskova, B.; Wilmanns, M.; Vanek, O.
Deposited on : 2023-09-22
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.5

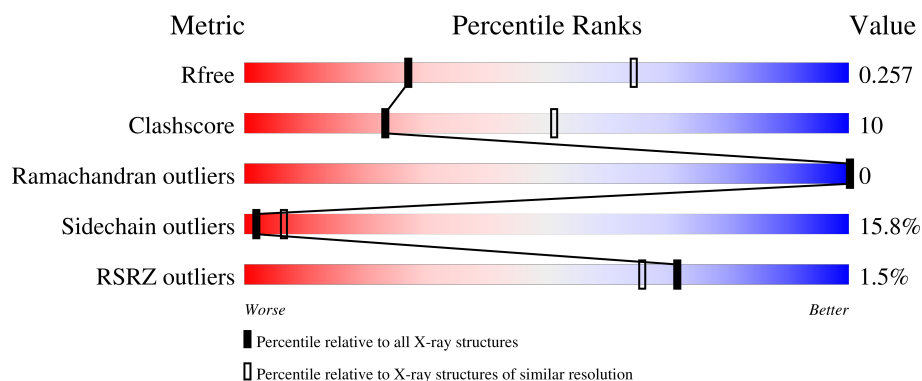
1 Overall quality at a glance

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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	182	<div> <div>2%</div> <div> <div>41%</div> <div>19%</div> <div>6%</div> <div>•</div> <div>32%</div> </div> </div>
1	B	182	<div> <div>46%</div> <div>15%</div> <div>7%</div> <div>•</div> <div>32%</div> </div>
1	C	182	<div> <div>2%</div> <div>45%</div> <div>16%</div> <div>5%</div> <div>•</div> <div>32%</div> </div>
1	D	182	<div> <div>•</div> <div>49%</div> <div>13%</div> <div>•</div> <div>33%</div> </div>
1	E	182	<div> <div>•</div> <div>45%</div> <div>17%</div> <div>6%</div> <div>32%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	182	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>48%14%6%32%</div></div>
1	G	182	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>43%18%5%34%</div></div>
1	H	182	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>45%18%5%32%</div></div>
1	I	182	<div><div><div></div><div></div><div></div><div></div></div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>43%18%7%32%</div></div>
1	J	182	<div><div><div></div><div></div><div></div><div></div></div><div></div><div><div></div><div></div><div></div><div></div></div><div>46%15%7%32%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10402 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 Killer cell lectin-like receptor subfamily F member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	123	Total	C	N	O	S	0	0	0
			1021	667	163	182	9			
1	D	122	Total	C	N	O	S	0	0	0
			1014	663	162	180	9			
1	A	123	Total	C	N	O	S	0	0	0
			1021	667	163	182	9			
1	B	124	Total	C	N	O	S	0	0	0
			1030	672	165	184	9			
1	E	124	Total	C	N	O	S	0	0	0
			1030	672	165	184	9			
1	F	124	Total	C	N	O	S	0	0	0
			1030	672	165	184	9			
1	G	121	Total	C	N	O	S	0	0	0
			1007	658	161	179	9			
1	H	123	Total	C	N	O	S	0	0	0
			1021	667	163	182	9			
1	I	123	Total	C	N	O	S	0	0	0
			1021	667	163	182	9			
1	J	123	Total	C	N	O	S	0	0	0
			1024	669	165	181	9			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ILE	-	expression tag	UNP Q9NZS2
C	2	THR	-	expression tag	UNP Q9NZS2
C	3	GLY	-	expression tag	UNP Q9NZS2
C	43	SER	CYS	engineered mutation	UNP Q9NZS2
C	172	GLY	-	expression tag	UNP Q9NZS2
C	173	THR	-	expression tag	UNP Q9NZS2
C	174	HIS	-	expression tag	UNP Q9NZS2
C	175	HIS	-	expression tag	UNP Q9NZS2
C	176	HIS	-	expression tag	UNP Q9NZS2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	177	HIS	-	expression tag	UNP Q9NZS2
C	178	HIS	-	expression tag	UNP Q9NZS2
C	179	HIS	-	expression tag	UNP Q9NZS2
C	180	HIS	-	expression tag	UNP Q9NZS2
C	181	HIS	-	expression tag	UNP Q9NZS2
C	182	GLY	-	expression tag	UNP Q9NZS2
D	1	ILE	-	expression tag	UNP Q9NZS2
D	2	THR	-	expression tag	UNP Q9NZS2
D	3	GLY	-	expression tag	UNP Q9NZS2
D	43	SER	CYS	engineered mutation	UNP Q9NZS2
D	172	GLY	-	expression tag	UNP Q9NZS2
D	173	THR	-	expression tag	UNP Q9NZS2
D	174	HIS	-	expression tag	UNP Q9NZS2
D	175	HIS	-	expression tag	UNP Q9NZS2
D	176	HIS	-	expression tag	UNP Q9NZS2
D	177	HIS	-	expression tag	UNP Q9NZS2
D	178	HIS	-	expression tag	UNP Q9NZS2
D	179	HIS	-	expression tag	UNP Q9NZS2
D	180	HIS	-	expression tag	UNP Q9NZS2
D	181	HIS	-	expression tag	UNP Q9NZS2
D	182	GLY	-	expression tag	UNP Q9NZS2
A	1	ILE	-	expression tag	UNP Q9NZS2
A	2	THR	-	expression tag	UNP Q9NZS2
A	3	GLY	-	expression tag	UNP Q9NZS2
A	43	SER	CYS	engineered mutation	UNP Q9NZS2
A	172	GLY	-	expression tag	UNP Q9NZS2
A	173	THR	-	expression tag	UNP Q9NZS2
A	174	HIS	-	expression tag	UNP Q9NZS2
A	175	HIS	-	expression tag	UNP Q9NZS2
A	176	HIS	-	expression tag	UNP Q9NZS2
A	177	HIS	-	expression tag	UNP Q9NZS2
A	178	HIS	-	expression tag	UNP Q9NZS2
A	179	HIS	-	expression tag	UNP Q9NZS2
A	180	HIS	-	expression tag	UNP Q9NZS2
A	181	HIS	-	expression tag	UNP Q9NZS2
A	182	GLY	-	expression tag	UNP Q9NZS2
B	1	ILE	-	expression tag	UNP Q9NZS2
B	2	THR	-	expression tag	UNP Q9NZS2
B	3	GLY	-	expression tag	UNP Q9NZS2
B	43	SER	CYS	engineered mutation	UNP Q9NZS2
B	172	GLY	-	expression tag	UNP Q9NZS2
B	173	THR	-	expression tag	UNP Q9NZS2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	174	HIS	-	expression tag	UNP Q9NZS2
B	175	HIS	-	expression tag	UNP Q9NZS2
B	176	HIS	-	expression tag	UNP Q9NZS2
B	177	HIS	-	expression tag	UNP Q9NZS2
B	178	HIS	-	expression tag	UNP Q9NZS2
B	179	HIS	-	expression tag	UNP Q9NZS2
B	180	HIS	-	expression tag	UNP Q9NZS2
B	181	HIS	-	expression tag	UNP Q9NZS2
B	182	GLY	-	expression tag	UNP Q9NZS2
E	1	ILE	-	expression tag	UNP Q9NZS2
E	2	THR	-	expression tag	UNP Q9NZS2
E	3	GLY	-	expression tag	UNP Q9NZS2
E	43	SER	CYS	engineered mutation	UNP Q9NZS2
E	172	GLY	-	expression tag	UNP Q9NZS2
E	173	THR	-	expression tag	UNP Q9NZS2
E	174	HIS	-	expression tag	UNP Q9NZS2
E	175	HIS	-	expression tag	UNP Q9NZS2
E	176	HIS	-	expression tag	UNP Q9NZS2
E	177	HIS	-	expression tag	UNP Q9NZS2
E	178	HIS	-	expression tag	UNP Q9NZS2
E	179	HIS	-	expression tag	UNP Q9NZS2
E	180	HIS	-	expression tag	UNP Q9NZS2
E	181	HIS	-	expression tag	UNP Q9NZS2
E	182	GLY	-	expression tag	UNP Q9NZS2
F	1	ILE	-	expression tag	UNP Q9NZS2
F	2	THR	-	expression tag	UNP Q9NZS2
F	3	GLY	-	expression tag	UNP Q9NZS2
F	43	SER	CYS	engineered mutation	UNP Q9NZS2
F	172	GLY	-	expression tag	UNP Q9NZS2
F	173	THR	-	expression tag	UNP Q9NZS2
F	174	HIS	-	expression tag	UNP Q9NZS2
F	175	HIS	-	expression tag	UNP Q9NZS2
F	176	HIS	-	expression tag	UNP Q9NZS2
F	177	HIS	-	expression tag	UNP Q9NZS2
F	178	HIS	-	expression tag	UNP Q9NZS2
F	179	HIS	-	expression tag	UNP Q9NZS2
F	180	HIS	-	expression tag	UNP Q9NZS2
F	181	HIS	-	expression tag	UNP Q9NZS2
F	182	GLY	-	expression tag	UNP Q9NZS2
G	1	ILE	-	expression tag	UNP Q9NZS2
G	2	THR	-	expression tag	UNP Q9NZS2
G	3	GLY	-	expression tag	UNP Q9NZS2

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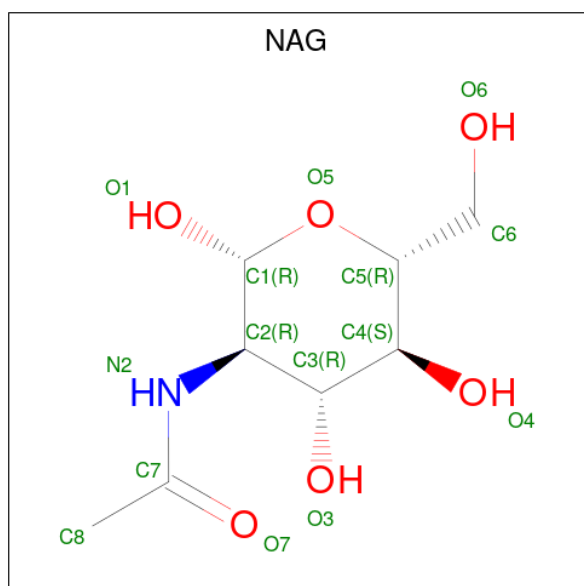
Chain	Residue	Modelled	Actual	Comment	Reference
G	43	SER	CYS	engineered mutation	UNP Q9NZS2
G	172	GLY	-	expression tag	UNP Q9NZS2
G	173	THR	-	expression tag	UNP Q9NZS2
G	174	HIS	-	expression tag	UNP Q9NZS2
G	175	HIS	-	expression tag	UNP Q9NZS2
G	176	HIS	-	expression tag	UNP Q9NZS2
G	177	HIS	-	expression tag	UNP Q9NZS2
G	178	HIS	-	expression tag	UNP Q9NZS2
G	179	HIS	-	expression tag	UNP Q9NZS2
G	180	HIS	-	expression tag	UNP Q9NZS2
G	181	HIS	-	expression tag	UNP Q9NZS2
G	182	GLY	-	expression tag	UNP Q9NZS2
H	1	ILE	-	expression tag	UNP Q9NZS2
H	2	THR	-	expression tag	UNP Q9NZS2
H	3	GLY	-	expression tag	UNP Q9NZS2
H	43	SER	CYS	engineered mutation	UNP Q9NZS2
H	172	GLY	-	expression tag	UNP Q9NZS2
H	173	THR	-	expression tag	UNP Q9NZS2
H	174	HIS	-	expression tag	UNP Q9NZS2
H	175	HIS	-	expression tag	UNP Q9NZS2
H	176	HIS	-	expression tag	UNP Q9NZS2
H	177	HIS	-	expression tag	UNP Q9NZS2
H	178	HIS	-	expression tag	UNP Q9NZS2
H	179	HIS	-	expression tag	UNP Q9NZS2
H	180	HIS	-	expression tag	UNP Q9NZS2
H	181	HIS	-	expression tag	UNP Q9NZS2
H	182	GLY	-	expression tag	UNP Q9NZS2
I	1	ILE	-	expression tag	UNP Q9NZS2
I	2	THR	-	expression tag	UNP Q9NZS2
I	3	GLY	-	expression tag	UNP Q9NZS2
I	43	SER	CYS	engineered mutation	UNP Q9NZS2
I	172	GLY	-	expression tag	UNP Q9NZS2
I	173	THR	-	expression tag	UNP Q9NZS2
I	174	HIS	-	expression tag	UNP Q9NZS2
I	175	HIS	-	expression tag	UNP Q9NZS2
I	176	HIS	-	expression tag	UNP Q9NZS2
I	177	HIS	-	expression tag	UNP Q9NZS2
I	178	HIS	-	expression tag	UNP Q9NZS2
I	179	HIS	-	expression tag	UNP Q9NZS2
I	180	HIS	-	expression tag	UNP Q9NZS2
I	181	HIS	-	expression tag	UNP Q9NZS2
I	182	GLY	-	expression tag	UNP Q9NZS2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1	ILE	-	expression tag	UNP Q9NZS2
J	2	THR	-	expression tag	UNP Q9NZS2
J	3	GLY	-	expression tag	UNP Q9NZS2
J	43	SER	CYS	engineered mutation	UNP Q9NZS2
J	172	GLY	-	expression tag	UNP Q9NZS2
J	173	THR	-	expression tag	UNP Q9NZS2
J	174	HIS	-	expression tag	UNP Q9NZS2
J	175	HIS	-	expression tag	UNP Q9NZS2
J	176	HIS	-	expression tag	UNP Q9NZS2
J	177	HIS	-	expression tag	UNP Q9NZS2
J	178	HIS	-	expression tag	UNP Q9NZS2
J	179	HIS	-	expression tag	UNP Q9NZS2
J	180	HIS	-	expression tag	UNP Q9NZS2
J	181	HIS	-	expression tag	UNP Q9NZS2
J	182	GLY	-	expression tag	UNP Q9NZS2

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



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		

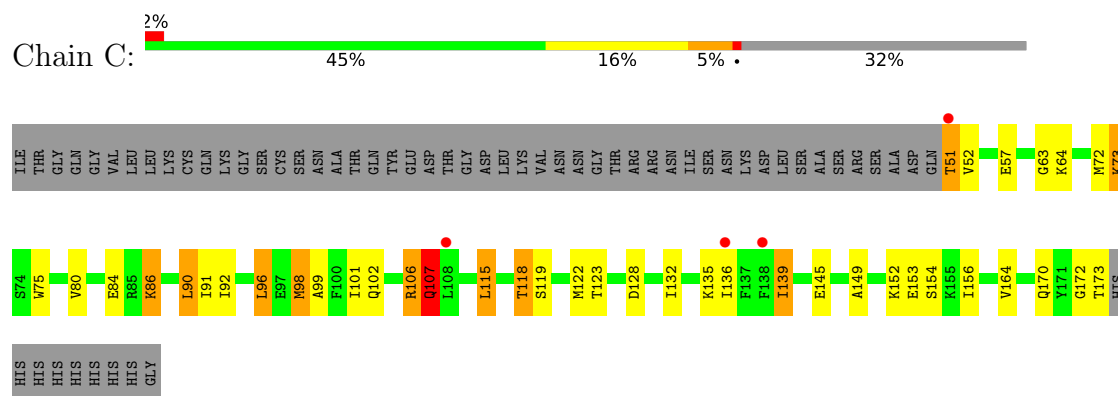
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	6	Total	O	0	0
			6	6		
3	D	8	Total	O	0	0
			8	8		
3	A	3	Total	O	0	0
			3	3		
3	B	3	Total	O	0	0
			3	3		
3	E	2	Total	O	0	0
			2	2		
3	F	3	Total	O	0	0
			3	3		
3	G	5	Total	O	0	0
			5	5		
3	H	3	Total	O	0	0
			3	3		
3	I	5	Total	O	0	0
			5	5		
3	J	5	Total	O	0	0
			5	5		

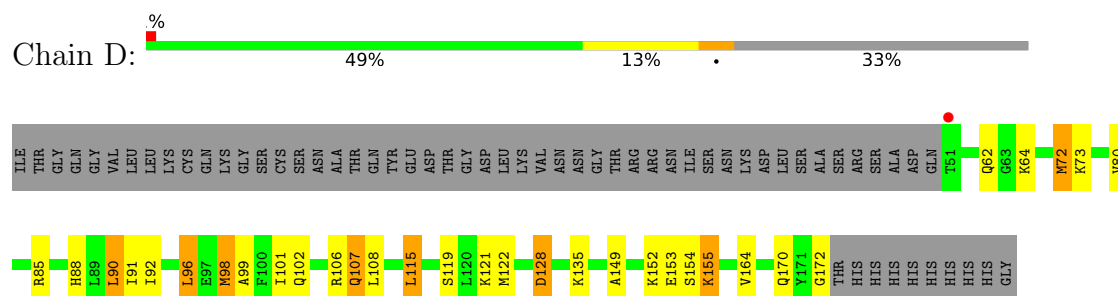
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

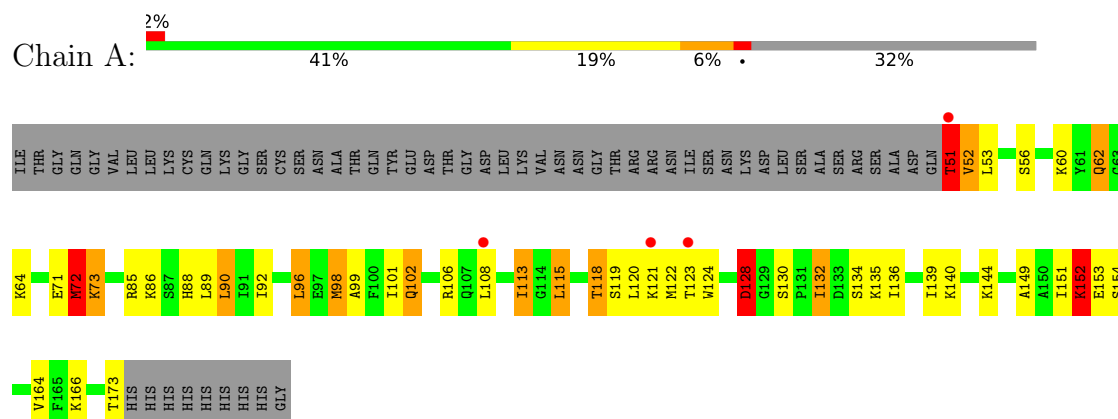
- Molecule 1: Killer cell lectin-like receptor subfamily F member 1



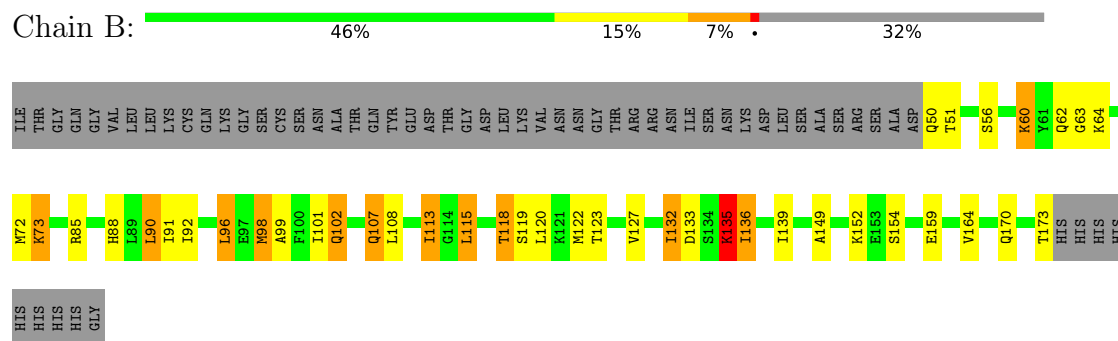
- Molecule 1: Killer cell lectin-like receptor subfamily F member 1



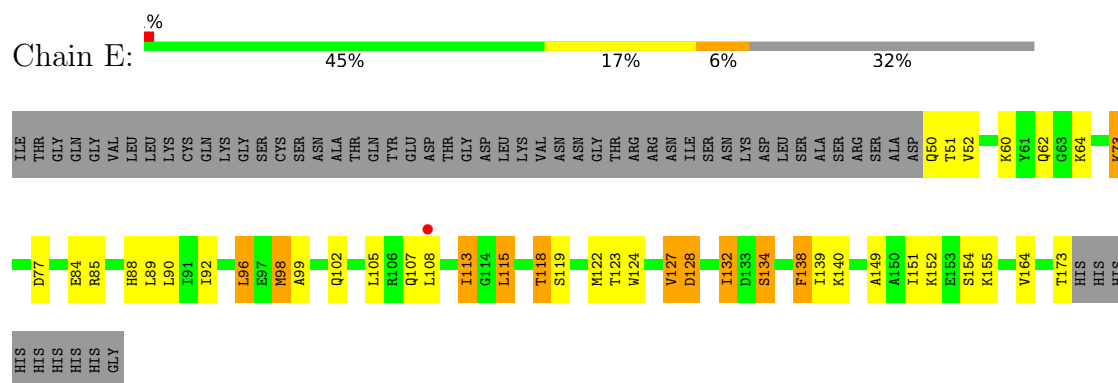
- Molecule 1: Killer cell lectin-like receptor subfamily F member 1



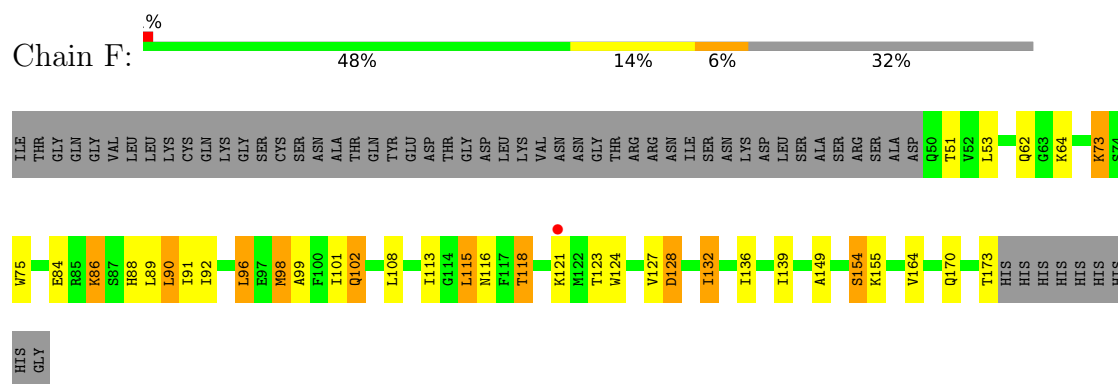
- Molecule 1: Killer cell lectin-like receptor subfamily F member 1



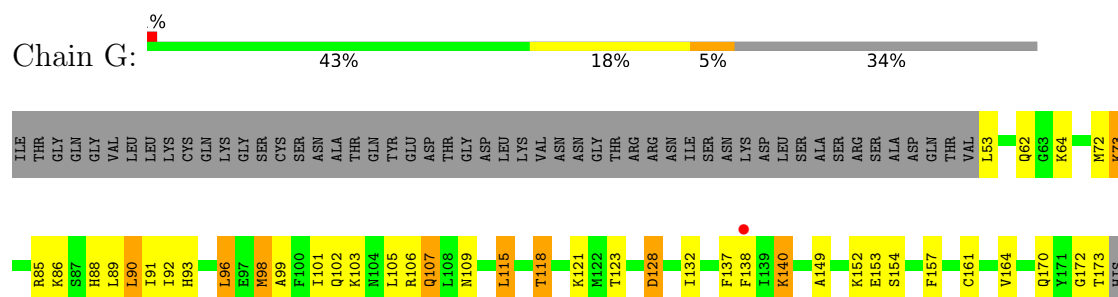
- Molecule 1: Killer cell lectin-like receptor subfamily F member 1



- Molecule 1: Killer cell lectin-like receptor subfamily F member 1



- Molecule 1: Killer cell lectin-like receptor subfamily F member 1



HIS
HIS
HIS
HIS
HIS
HIS
HIS
GLY

- Molecule 1: Killer cell lectin-like receptor subfamily F member 1



ILE THR GLN LYS CYS GLN LYS SER CYS ASN ALA THR GLN TYR ASP THR GLY ASP LEU LYS VAL ASN ASN GLY THR ARG ARG ASN ILE SER ASN LYS ASP LEU SER ALA SER ARG SER ALA ASP ASP GLN T51 V52 Q62 G63 K64 K73 R85

H88 L89 L90 L91 I92 I93 L96 E97 M98 A99 F100 I101 Q102 R106 Q107 L108 I113 G114 L115 T118 S119 L120 K121 M122 T123 W124 V127 D128 I132 I135 F138 I139 K144 E145 A149 A150 I151 K152 E153 S154 V164 Q170 T173 HIS HIS HIS HIS

HIS
HIS
HIS
HIS
HIS
GLY

- Molecule 1: Killer cell lectin-like receptor subfamily F member 1



ILE THR GLN LYS CYS GLN LYS SER CYS ASN ALA THR GLN TYR ASP THR GLY ASP LEU LYS VAL ASN ASN GLY THR ARG ARG ASN ILE SER ASN LYS ASP LEU SER ALA SER ARG SER ALA ASP ASP GLN T51 Q62 G63 K64 K73 S76

V80 R85 K86 S87 H88 L89 L90 L91 I92 L96 E97 M98 A99 F100 I101 Q102 K103 N104 R106 Q107 L108 I113 G114 L115 T118 S119 M122 T123 W124 I132 I136 F137 F138 I139 K140 G141 P142 A143 K144 E145 A149 A150 I151 K152 E153 S154 K155 I156 V164

Q170 T173 HIS HIS HIS HIS HIS HIS HIS GLY

- Molecule 1: Killer cell lectin-like receptor subfamily F member 1



ILE THR GLN LYS CYS GLN LYS SER CYS ASN ALA THR GLN TYR ASP THR GLY ASP LEU LYS VAL ASN ASN GLY THR ARG ARG ASN ILE SER ASN LYS ASP LEU SER ALA SER ARG SER ALA ASP ASP GLN T51 V52 L59 Q62 G63 K64 E71

M72 K73 V80 R85 H88 L89 L90 L91 I92 L96 E97 M98 A99 F100 I101 Q102 K103 R106 Q107 L108 T113 G114 L115 T118 T123 W124 V127 D128 T132 K135 I139 A149 K152 E153 S154 V164 F165 K166 G172 T173 H174 HIS HIS HIS HIS

HIS
HIS
HIS
GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	183.54Å 183.54Å 123.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.61 – 2.90 97.61 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.9 (97.61-2.90) 93.9 (97.61-2.90)	Depositor EDS
R_{merge}	0.64	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.221 , 0.257 0.221 , 0.257	Depositor DCC
R_{free} test set	2340 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 102.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10402	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.61	0/1051	1.21	9/1420 (0.6%)
1	B	0.62	0/1060	1.12	4/1432 (0.3%)
1	C	0.65	0/1051	1.25	6/1420 (0.4%)
1	D	0.65	1/1044 (0.1%)	1.20	5/1410 (0.4%)
1	E	0.66	1/1060 (0.1%)	1.20	4/1432 (0.3%)
1	F	0.71	1/1060 (0.1%)	1.32	7/1432 (0.5%)
1	G	0.65	0/1037	1.18	4/1400 (0.3%)
1	H	0.58	0/1051	1.10	3/1420 (0.2%)
1	I	0.57	0/1051	1.17	4/1420 (0.3%)
1	J	0.62	0/1055	1.19	8/1425 (0.6%)
All	All	0.63	3/10520 (0.0%)	1.19	54/14211 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	G	0	1
1	I	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	84	GLU	CD-OE1	6.69	1.33	1.25
1	D	172	GLY	C-O	6.45	1.33	1.23
1	E	84	GLU	CD-OE2	6.19	1.32	1.25

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	116	ASN	N-CA-CB	-13.45	86.40	110.60
1	F	116	ASN	CB-CA-C	-13.00	84.40	110.40
1	A	62	GLN	CB-CA-C	8.76	127.91	110.40
1	C	128	ASP	CB-CA-C	-8.75	92.90	110.40
1	E	173	THR	CA-CB-OG1	8.27	126.37	109.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51	THR	Peptide
1	D	106	ARG	Sidechain
1	G	172	GLY	Peptide
1	I	137	PHE	Peptide

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	1021	0	994	27	0
1	B	1030	0	1002	23	0
1	C	1021	0	994	28	0
1	D	1014	0	987	21	0
1	E	1030	0	1002	22	0
1	F	1030	0	1002	19	0
1	G	1007	0	978	21	0
1	H	1021	0	994	19	0
1	I	1021	0	994	25	0
1	J	1024	0	994	20	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	1	0
2	D	14	0	13	1	0
2	E	14	0	13	1	0
2	F	14	0	13	2	0
2	G	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	14	0	13	1	0
2	I	14	0	13	0	0
2	J	14	0	13	1	0
3	A	3	0	0	1	0
3	B	3	0	0	0	0
3	C	6	0	0	0	0
3	D	8	0	0	7	0
3	E	2	0	0	1	0
3	F	3	0	0	0	0
3	G	5	0	0	2	0
3	H	3	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	1	0
All	All	10402	0	10071	207	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.

The worst 5 of 207 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:D:128:ASP:HA	3:D:305:HOH:O	1.55	1.04
1:I:102:GLN:OE1	1:I:154:SER:HB3	1.64	0.96
1:G:161:CYS:HB2	3:G:303:HOH:O	1.68	0.94
1:F:102:GLN:OE1	1:F:154:SER:HB3	1.69	0.91
1:J:102:GLN:OE1	1:J:154:SER:HB3	1.70	0.89

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	121/182 (66%)	116 (96%)	5 (4%)	0	100	100
1	B	122/182 (67%)	117 (96%)	5 (4%)	0	100	100
1	C	121/182 (66%)	118 (98%)	3 (2%)	0	100	100
1	D	120/182 (66%)	116 (97%)	4 (3%)	0	100	100
1	E	122/182 (67%)	117 (96%)	5 (4%)	0	100	100
1	F	122/182 (67%)	118 (97%)	4 (3%)	0	100	100
1	G	119/182 (65%)	117 (98%)	2 (2%)	0	100	100
1	H	121/182 (66%)	116 (96%)	5 (4%)	0	100	100
1	I	121/182 (66%)	115 (95%)	6 (5%)	0	100	100
1	J	121/182 (66%)	116 (96%)	5 (4%)	0	100	100
All	All	1210/1820 (66%)	1166 (96%)	44 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	114/164 (70%)	89 (78%)	25 (22%)	1	2
1	B	115/164 (70%)	94 (82%)	21 (18%)	1	4
1	C	114/164 (70%)	98 (86%)	16 (14%)	3	9
1	D	113/164 (69%)	101 (89%)	12 (11%)	5	18
1	E	115/164 (70%)	96 (84%)	19 (16%)	2	6
1	F	115/164 (70%)	97 (84%)	18 (16%)	2	7
1	G	112/164 (68%)	96 (86%)	16 (14%)	2	8
1	H	114/164 (70%)	99 (87%)	15 (13%)	3	10
1	I	114/164 (70%)	95 (83%)	19 (17%)	2	5
1	J	114/164 (70%)	95 (83%)	19 (17%)	2	5
All	All	1140/1640 (70%)	960 (84%)	180 (16%)	2	6

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	98	MET
1	I	64	LYS
1	G	109	ASN
1	H	90	LEU
1	I	113	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	102	GLN
1	J	88	HIS
1	F	95	GLN
1	J	107	GLN
1	H	170	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	201	1	14,14,15	0.68	0	17,19,21	2.40	6 (35%)
2	NAG	G	201	1	14,14,15	0.54	0	17,19,21	2.01	4 (23%)
2	NAG	H	201	1	14,14,15	0.63	0	17,19,21	1.61	3 (17%)
2	NAG	F	201	1	14,14,15	0.76	0	17,19,21	2.78	7 (41%)
2	NAG	I	201	1	14,14,15	0.68	1 (7%)	17,19,21	2.48	2 (11%)
2	NAG	A	201	1	14,14,15	0.50	0	17,19,21	2.70	6 (35%)
2	NAG	C	201	1	14,14,15	0.64	0	17,19,21	3.30	7 (41%)
2	NAG	B	201	1	14,14,15	0.54	0	17,19,21	2.62	3 (17%)
2	NAG	J	201	1	14,14,15	0.56	0	17,19,21	2.63	6 (35%)
2	NAG	D	201	1	14,14,15	0.45	0	17,19,21	2.86	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	201	1	-	4/6/23/26	0/1/1/1
2	NAG	G	201	1	-	4/6/23/26	0/1/1/1
2	NAG	H	201	1	-	4/6/23/26	0/1/1/1
2	NAG	F	201	1	-	3/6/23/26	0/1/1/1
2	NAG	I	201	1	-	2/6/23/26	0/1/1/1
2	NAG	A	201	1	-	5/6/23/26	0/1/1/1
2	NAG	C	201	1	-	4/6/23/26	0/1/1/1
2	NAG	B	201	1	-	2/6/23/26	0/1/1/1
2	NAG	J	201	1	-	4/6/23/26	0/1/1/1
2	NAG	D	201	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	201	NAG	C1-C2	2.14	1.55	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	201	NAG	C1-C2-N2	9.39	126.53	110.49
2	B	201	NAG	C1-C2-N2	8.92	125.72	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	NAG	C2-N2-C7	8.25	134.65	122.90
2	D	201	NAG	O5-C1-C2	7.65	123.37	111.29
2	C	201	NAG	O4-C4-C3	-7.27	93.55	110.35

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	NAG	C8-C7-N2-C2
2	C	201	NAG	O7-C7-N2-C2
2	A	201	NAG	C8-C7-N2-C2
2	A	201	NAG	O7-C7-N2-C2
2	B	201	NAG	C8-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	201	NAG	1	0
2	H	201	NAG	1	0
2	F	201	NAG	2	0
2	C	201	NAG	1	0
2	J	201	NAG	1	0
2	D	201	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	123/182 (67%)	-0.08	4 (3%) 49 43	55, 100, 166, 191	0
1	B	124/182 (68%)	-0.21	0 100 100	62, 111, 166, 184	0
1	C	123/182 (67%)	-0.35	4 (3%) 49 43	45, 78, 147, 172	0
1	D	122/182 (67%)	-0.54	1 (0%) 82 78	47, 78, 131, 152	0
1	E	124/182 (68%)	-0.43	1 (0%) 82 78	40, 80, 152, 188	0
1	F	124/182 (68%)	-0.41	1 (0%) 82 78	46, 79, 142, 171	0
1	G	121/182 (66%)	-0.46	1 (0%) 82 78	49, 82, 139, 193	0
1	H	123/182 (67%)	-0.16	2 (1%) 70 64	63, 106, 165, 188	0
1	I	123/182 (67%)	-0.07	4 (3%) 49 43	61, 106, 168, 202	0
1	J	123/182 (67%)	-0.31	0 100 100	49, 88, 147, 170	0
All	All	1230/1820 (67%)	-0.30	18 (1%) 71 66	40, 90, 160, 202	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	121	LYS	4.1
1	C	51	THR	3.8
1	C	108	LEU	3.4
1	C	138	PHE	3.3
1	E	108	LEU	3.3

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	H	201	14/15	0.92	0.08	79,90,99,102	0
2	NAG	E	201	14/15	0.93	0.09	76,87,102,114	0
2	NAG	J	201	14/15	0.93	0.07	80,93,112,120	0
2	NAG	D	201	14/15	0.94	0.09	73,92,128,133	0
2	NAG	C	201	14/15	0.95	0.07	71,85,106,110	0
2	NAG	G	201	14/15	0.95	0.07	74,83,114,126	0
2	NAG	F	201	14/15	0.96	0.07	54,71,97,101	0
2	NAG	B	201	14/15	0.96	0.06	69,77,109,113	0
2	NAG	I	201	14/15	0.97	0.06	81,95,106,108	0
2	NAG	A	201	14/15	0.97	0.06	73,81,96,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.