



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2022 – 08:11 PM JST

PDB ID : 7FI7
Title : Crystal structure of human MICA mutants in complex with natural killer cell receptor NKG2D
Authors : Cai, W.; Peng, S.; Xu, T.; Tian, Y.; Li, Y.; Liu, J.
Deposited on : 2021-07-30
Resolution : 2.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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
Xtriage (Phenix)	:	1.13
EDS	:	2.30
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)	:	2.30

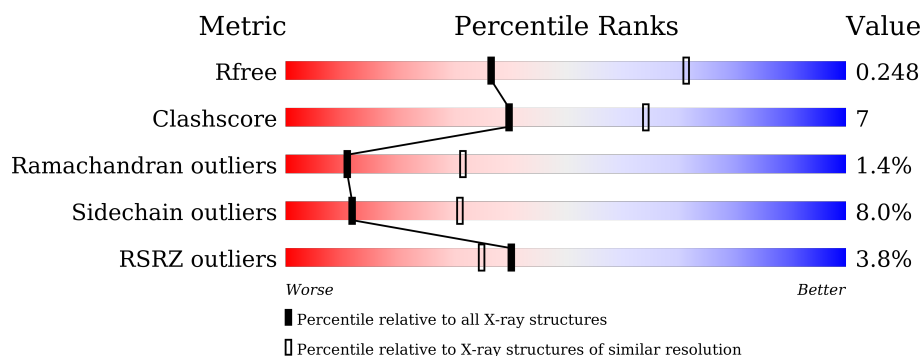
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	139	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	139	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>•</div> <div>•</div> </div> </div>
2	C	275	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>•</div> <div>•</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4231 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 NKG2-D type II integral membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			1004	638	161	193	12			
1	B	133	Total	C	N	O	S	0	0	0
			1076	683	173	208	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	MET	-	initiating methionine	UNP P26718
A	79	GLU	-	expression tag	UNP P26718
B	78	MET	-	initiating methionine	UNP P26718
B	79	GLU	-	expression tag	UNP P26718

- Molecule 2 is a protein called MHC class I polypeptide-related sequence A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	264	Total	C	N	O	S	0	0	0
			2145	1328	396	405	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP Q29983
C	14	MET	SER	engineered mutation	UNP Q29983
C	109	ILE	GLN	engineered mutation	UNP Q29983
C	121	GLY	GLN	engineered mutation	UNP Q29983
C	147	TRP	LEU	engineered mutation	UNP Q29983
C	158	TRP	TYR	engineered mutation	UNP Q29983

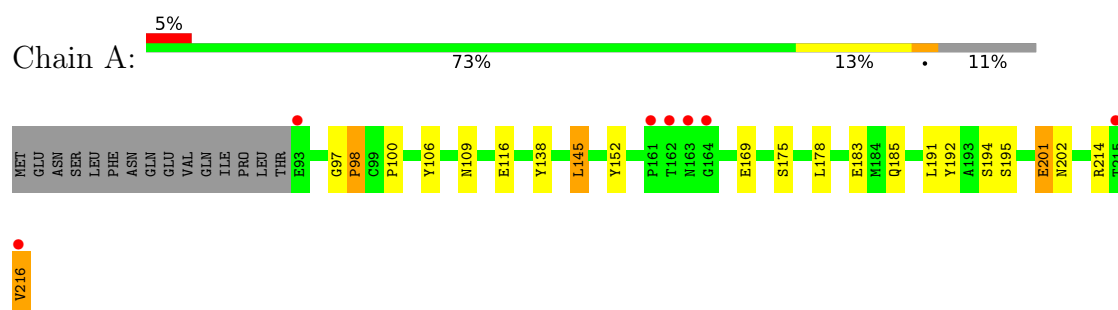
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	B	1	Total 1	O 1	0	0
3	C	4	Total 4	O 4	0	0

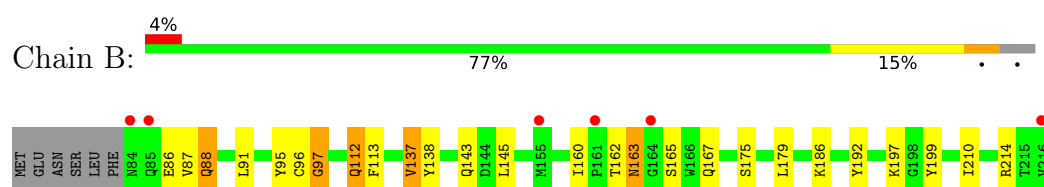
3 Residue-property plots [i](#)

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.

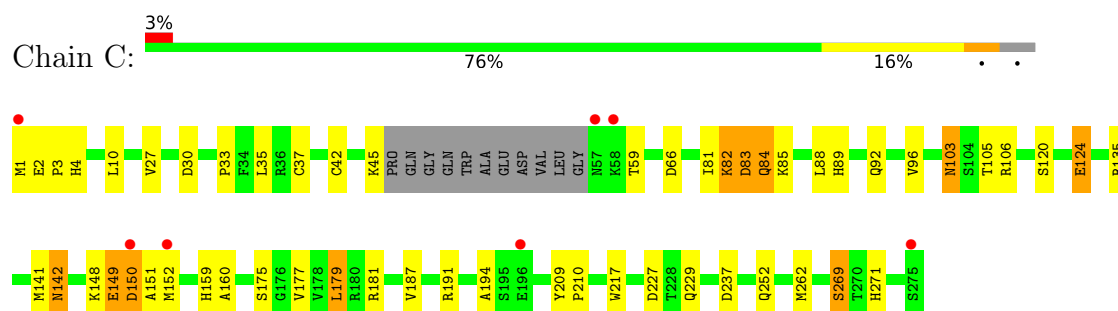
- Molecule 1: NKG2-D type II integral membrane protein



- Molecule 1: NKG2-D type II integral membrane protein



- Molecule 2: MHC class I polypeptide-related sequence A



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.25Å 124.25Å 184.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 2.78 19.83 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.83-2.78) 99.8 (19.83-2.78)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.192 , 0.246 0.195 , 0.248	Depositor DCC
R_{free} test set	902 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.002 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4231	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.69	0/1032	0.88	1/1398 (0.1%)
1	B	0.69	0/1105	0.83	0/1499
2	C	0.70	0/2197	0.90	0/2972
All	All	0.69	0/4334	0.88	1/5869 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	GLU	CB-CA-C	-5.92	98.56	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1004	0	942	14	0
1	B	1076	0	1015	25	0
2	C	2145	0	2046	26	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	4	0	0	1	0
All	All	4231	0	4003	60	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 7.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:237:ASP:HB3	3:C:301:HOH:O	1.48	1.13
1:B:160:ILE:HD11	1:B:167:GLN:HE21	1.32	0.94
1:B:112:GLN:HE21	1:B:113:PHE:H	1.16	0.90
2:C:217:TRP:H	2:C:229:GLN:HE22	1.25	0.83
1:B:160:ILE:CD1	1:B:167:GLN:HE21	1.98	0.77
2:C:269:SER:HG	2:C:271:HIS:HE2	1.22	0.74
1:B:112:GLN:HE21	1:B:113:PHE:N	1.86	0.73
1:B:88:GLN:HE21	1:B:88:GLN:HA	1.53	0.72
2:C:149:GLU:O	2:C:151:ALA:N	2.23	0.72
1:A:100:PRO:HB3	1:B:88:GLN:HE22	1.54	0.72
1:B:138:TYR:H	1:B:143:GLN:HE22	1.39	0.69
1:B:160:ILE:HD11	1:B:167:GLN:NE2	2.08	0.67
1:B:163:ASN:HD22	1:B:165:SER:H	1.43	0.64
1:B:138:TYR:H	1:B:143:GLN:NE2	1.96	0.62
1:A:100:PRO:HB3	1:B:88:GLN:NE2	2.16	0.59
1:A:185:GLN:HE21	1:A:202:ASN:H	1.48	0.59
1:A:183:GLU:O	2:C:82:LYS:NZ	2.36	0.58
2:C:148:LYS:O	2:C:150:ASP:N	2.37	0.57
1:A:98:PRO:HD3	1:B:95:TYR:CZ	2.39	0.57
1:B:163:ASN:ND2	1:B:165:SER:OG	2.38	0.56
2:C:83:ASP:N	2:C:83:ASP:OD1	2.38	0.56
1:A:191:LEU:HD11	1:A:201:GLU:HG3	1.89	0.55
1:B:137:VAL:HA	1:B:143:GLN:HE22	1.71	0.55
2:C:217:TRP:H	2:C:229:GLN:NE2	1.98	0.54
1:A:109:ASN:ND2	1:A:138:TYR:OH	2.39	0.53
1:B:112:GLN:NE2	1:B:112:GLN:HA	2.23	0.53
1:B:197:LYS:HE3	1:B:199:TYR:OH	2.08	0.53
1:B:112:GLN:NE2	1:B:113:PHE:H	1.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ILE:CD1	1:B:167:GLN:NE2	2.69	0.51
2:C:209:TYR:CG	2:C:210:PRO:HA	2.46	0.50
1:B:137:VAL:HG21	1:B:179:LEU:HD21	1.93	0.50
2:C:187:VAL:HG22	2:C:262:MET:HE1	1.92	0.50
1:B:199:TYR:CE2	2:C:160:ALA:HB1	2.46	0.50
1:B:138:TYR:N	1:B:143:GLN:HE22	2.09	0.50
2:C:179:LEU:N	2:C:179:LEU:HD23	2.29	0.47
2:C:175:SER:OG	2:C:177:VAL:CG2	2.63	0.47
2:C:10:LEU:O	2:C:92:GLN:HA	2.16	0.46
2:C:27:VAL:HB	2:C:35:LEU:HB2	1.98	0.45
1:B:96:CYS:O	1:B:97:GLY:O	2.35	0.45
1:A:175:SER:HB2	1:A:178:LEU:HD12	1.99	0.45
1:A:106:TYR:CD2	1:A:145:LEU:HG	2.51	0.44
1:B:88:GLN:HE21	1:B:88:GLN:CA	2.26	0.43
1:B:113:PHE:CD2	1:B:210:ILE:HG12	2.54	0.43
2:C:103:ASN:HD22	2:C:103:ASN:HA	1.51	0.43
2:C:37:CYS:HA	2:C:42:CYS:HA	2.01	0.42
1:A:194:SER:HA	1:A:195:SER:HA	1.72	0.42
2:C:84:GLN:NE2	2:C:89:HIS:CE1	2.88	0.41
1:A:214:ARG:HG3	1:A:216:VAL:HG13	2.02	0.41
2:C:217:TRP:HB2	2:C:229:GLN:NE2	2.35	0.41
2:C:141:MET:O	2:C:142:ASN:C	2.59	0.41
1:A:178:LEU:HD23	1:A:178:LEU:HA	1.98	0.41
1:B:192:TYR:CD2	1:B:192:TYR:C	2.94	0.41
2:C:149:GLU:C	2:C:151:ALA:H	2.23	0.41
2:C:33:PRO:HB2	2:C:45:LYS:CE	2.51	0.41
2:C:135:ARG:HA	2:C:135:ARG:HD2	1.92	0.41
1:A:214:ARG:HD2	1:A:214:ARG:HA	1.78	0.40
1:A:192:TYR:CD2	1:A:192:TYR:C	2.95	0.40
2:C:2:GLU:HB2	2:C:3:PRO:HD2	2.04	0.40
2:C:4:HIS:HA	2:C:30:ASP:OD1	2.22	0.40
2:C:105:THR:OG1	2:C:124:GLU:OE2	2.36	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	122/139 (88%)	115 (94%)	6 (5%)	1 (1%)	19	47
1	B	131/139 (94%)	122 (93%)	8 (6%)	1 (1%)	19	47
2	C	260/275 (94%)	239 (92%)	16 (6%)	5 (2%)	8	23
All	All	513/553 (93%)	476 (93%)	30 (6%)	7 (1%)	11	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	149	GLU
2	C	150	ASP
1	B	97	GLY
2	C	152	MET
2	C	194	ALA
1	A	98	PRO
2	C	81	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	114/129 (88%)	109 (96%)	5 (4%)	28	58
1	B	123/129 (95%)	111 (90%)	12 (10%)	8	21
2	C	237/245 (97%)	216 (91%)	21 (9%)	9	26
All	All	474/503 (94%)	436 (92%)	38 (8%)	12	31

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	GLU
1	A	145	LEU

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Mol	Chain	Res	Type
1	A	152	TYR
1	A	169	GLU
1	A	216	VAL
1	B	86	GLU
1	B	87	VAL
1	B	88	GLN
1	B	91	LEU
1	B	112	GLN
1	B	137	VAL
1	B	145	LEU
1	B	162	THR
1	B	163	ASN
1	B	175	SER
1	B	186	LYS
1	B	214	ARG
2	C	1	MET
2	C	59	THR
2	C	66	ASP
2	C	82	LYS
2	C	83	ASP
2	C	84	GLN
2	C	85	LYS
2	C	88	LEU
2	C	96	VAL
2	C	103	ASN
2	C	106	ARG
2	C	120	SER
2	C	124	GLU
2	C	142	ASN
2	C	159	HIS
2	C	179	LEU
2	C	181	ARG
2	C	191	ARG
2	C	227	ASP
2	C	252	GLN
2	C	269	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	109	ASN

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Mol	Chain	Res	Type
1	A	185	GLN
1	A	207	ASN
1	B	88	GLN
1	B	112	GLN
1	B	130	GLN
1	B	143	GLN
1	B	163	ASN
1	B	167	GLN
1	B	185	GLN
1	B	207	ASN
2	C	84	GLN
2	C	103	ASN
2	C	142	ASN
2	C	198	ASN
2	C	219	GLN
2	C	229	GLN
2	C	264	HIS
2	C	268	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	124/139 (89%)	-0.16	7 (5%)	24 19	48, 60, 117, 180	0
1	B	133/139 (95%)	-0.08	6 (4%)	33 27	50, 70, 123, 152	0
2	C	264/275 (96%)	-0.28	7 (2%)	54 49	41, 67, 115, 150	0
All	All	521/553 (94%)	-0.20	20 (3%)	40 35	41, 66, 117, 180	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	216	VAL	4.8
1	A	162	THR	4.8
1	A	164	GLY	4.1
1	A	93	GLU	3.9
1	A	161	PRO	3.8
2	C	150	ASP	3.4
1	A	216	VAL	3.2
1	B	161	PRO	3.0
2	C	58	LYS	2.7
2	C	152	MET	2.7
2	C	275	SER	2.7
1	A	163	ASN	2.6
1	B	85	GLN	2.6
1	A	215	THR	2.3
2	C	196	GLU	2.3
1	B	84	ASN	2.2
1	B	164	GLY	2.2
2	C	57	ASN	2.2
2	C	1	MET	2.1
1	B	155	MET	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.