



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2022 – 08:11 PM JST

PDB ID : 7FI5
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 : 2.39 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

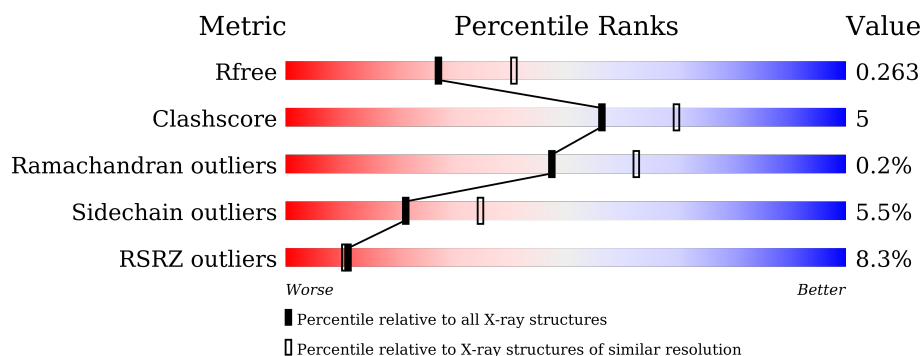
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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>9%</div> <div>81%</div> <div>7%</div> <div>11%</div> </div>
1	B	139	<div> <div>12%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
2	C	275	<div> <div>5%</div> <div>78%</div> <div>16%</div> <div>• 5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	302	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4247 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	261	Total	C	N	O	S	0	0	0
			2124	1316	392	402	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP Q29983
C	108	HIS	GLN	engineered mutation	UNP Q29983
C	120	TRP	GLN	engineered mutation	UNP Q29983
C	127	PHE	TRP	engineered mutation	UNP Q29983
C	146	TRP	LEU	engineered mutation	UNP Q29983
C	157	PHE	TYR	engineered mutation	UNP Q29983

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

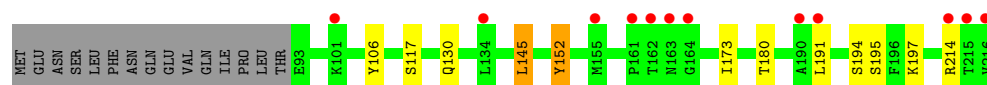
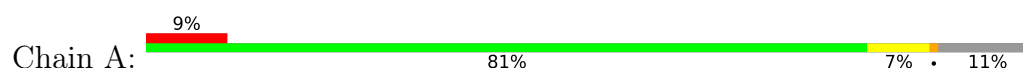
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	5	Total	O	0	0
			5	5		
4	C	13	Total	O	0	0
			13	13		

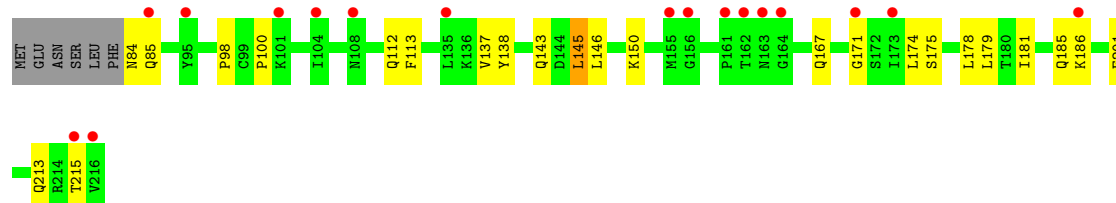
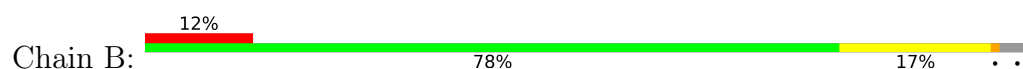
3 Residue-property plots [i](#)

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.

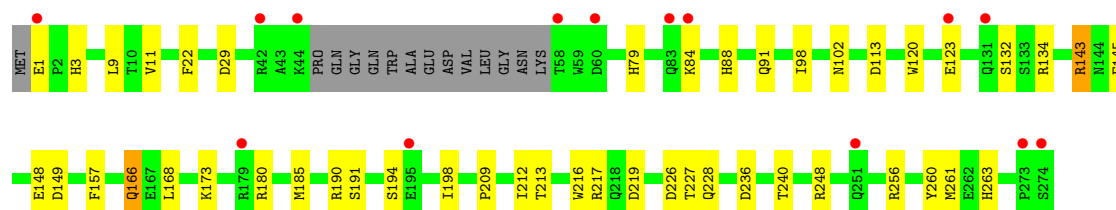
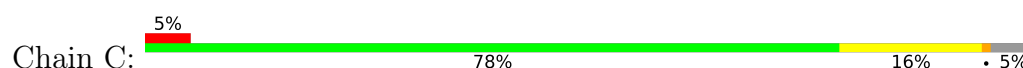
- Molecule 1: NKG2-D type II integral membrane protein



- 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	123.38Å 123.38Å 180.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 2.39 19.64 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.83-2.39) 99.3 (19.64-2.39)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.195 , 0.258 0.200 , 0.263	Depositor DCC
R_{free} test set	1279 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.016 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.000 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	0.96	EDS
Total number of atoms	4247	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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](#)

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

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	0.66	0/1032	0.82	0/1398
1	B	0.65	0/1105	0.78	0/1499
2	C	0.65	0/2177	0.86	0/2946
All	All	0.65	0/4314	0.83	0/5843

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1004	0	942	6	0
1	B	1076	0	1015	17	0
2	C	2124	0	2015	20	0
3	A	12	0	16	0	0
3	B	6	0	8	1	0
4	A	7	0	0	1	0
4	B	5	0	0	0	0
4	C	13	0	0	2	0
All	All	4247	0	3996	41	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.

All (41) 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:143:ARG:NH1	4:C:301:HOH:O	2.11	0.82
1:B:100:PRO:HD3	1:B:213:GLN:NE2	2.05	0.71
1:B:100:PRO:HD3	1:B:213:GLN:HE22	1.58	0.69
1:A:173:ILE:O	1:A:173:ILE:HD12	1.96	0.66
2:C:219:ASP:OD2	2:C:256:ARG:NH2	2.30	0.64
1:B:138:TYR:H	1:B:143:GLN:NE2	1.97	0.62
1:B:138:TYR:H	1:B:143:GLN:HE22	1.46	0.62
2:C:11:VAL:HG12	2:C:22:PHE:HB3	1.86	0.57
1:B:150:LYS:NZ	2:C:149:ASP:O	2.38	0.57
1:B:185:GLN:HG3	1:B:201:GLU:OE2	2.05	0.57
2:C:216:TRP:H	2:C:228:GLN:NE2	2.06	0.54
2:C:209:PRO:O	2:C:263:HIS:HE1	1.91	0.54
2:C:217:ARG:HD2	2:C:260:TYR:HB2	1.89	0.54
1:B:179:LEU:O	3:B:301:GOL:H2	2.09	0.52
2:C:216:TRP:H	2:C:228:GLN:HE22	1.56	0.52
1:B:137:VAL:HA	1:B:143:GLN:HE22	1.76	0.51
1:B:112:GLN:HE21	1:B:113:PHE:H	1.59	0.51
2:C:120:TRP:CZ3	2:C:157:PHE:HB3	2.47	0.49
1:A:117:SER:OG	4:A:401:HOH:O	2.18	0.49
2:C:9:LEU:O	2:C:91:GLN:HA	2.13	0.48
1:B:145:LEU:HD12	1:B:146:LEU:N	2.28	0.48
2:C:143:ARG:CG	2:C:143:ARG:HH11	2.27	0.48
1:B:174:LEU:CD2	1:B:181:ILE:HD11	2.45	0.47
2:C:79:HIS:CD2	2:C:145:PHE:CD1	3.04	0.46
1:A:152:TYR:CD1	1:A:191:LEU:HD13	2.50	0.46
1:B:98:PRO:O	1:B:215:THR:HG22	2.17	0.45
1:A:180:THR:HB	1:A:197:LYS:HD2	1.99	0.45
1:B:175:SER:HB2	1:B:178:LEU:HD12	2.00	0.44
1:B:181:ILE:O	2:C:166:GLN:NE2	2.51	0.43
1:A:106:TYR:CD2	1:A:145:LEU:HG	2.54	0.43
1:A:194:SER:HA	1:A:195:SER:HA	1.82	0.43
2:C:213:THR:O	2:C:261:MET:HA	2.19	0.43
1:B:167:GLN:NE2	1:B:171:GLY:HA2	2.35	0.42
2:C:3:HIS:HA	2:C:29:ASP:OD1	2.20	0.42
1:B:174:LEU:HD21	1:B:181:ILE:HD11	2.01	0.42
2:C:212:ILE:O	4:C:302:HOH:O	2.22	0.41
2:C:236:ASP:OD1	2:C:240:THR:C	2.58	0.41
1:B:178:LEU:HD23	1:B:178:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:HIS:HA	2:C:113:ASP:OD1	2.20	0.41
2:C:98:ILE:HG13	2:C:168:LEU:HD23	2.03	0.41
2:C:143:ARG:HH11	2:C:143:ARG:HG2	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	122/139 (88%)	118 (97%)	4 (3%)	0	100	100
1	B	131/139 (94%)	126 (96%)	5 (4%)	0	100	100
2	C	257/275 (94%)	243 (95%)	13 (5%)	1 (0%)	34	48
All	All	510/553 (92%)	487 (96%)	22 (4%)	1 (0%)	47	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	132	SER

5.3.2 Protein sidechains [i](#)

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%)	110 (96%)	4 (4%)	36	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	123/129 (95%)	119 (97%)	4 (3%)	38	57
2	C	235/246 (96%)	217 (92%)	18 (8%)	13	20
All	All	472/504 (94%)	446 (94%)	26 (6%)	21	35

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	145	LEU
1	A	152	TYR
1	A	214	ARG
1	B	84	ASN
1	B	85	GLN
1	B	145	LEU
1	B	186	LYS
2	C	1	GLU
2	C	84	LYS
2	C	102	ASN
2	C	123	GLU
2	C	134	ARG
2	C	143	ARG
2	C	148	GLU
2	C	166	GLN
2	C	173	LYS
2	C	180	ARG
2	C	185	MET
2	C	190	ARG
2	C	191	SER
2	C	194	SER
2	C	198	ILE
2	C	226	ASP
2	C	227	THR
2	C	248	ARG

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	167	GLN
1	A	185	GLN

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Mol	Chain	Res	Type
1	A	207	ASN
1	B	84	ASN
1	B	88	GLN
1	B	112	GLN
1	B	130	GLN
1	B	143	GLN
1	B	167	GLN
1	B	213	GLN
2	C	102	ASN
2	C	109	HIS
2	C	136	GLN
2	C	161	HIS
2	C	197	ASN
2	C	228	GLN
2	C	238	ASN
2	C	263	HIS
2	C	267	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](#)

3 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	GOL	A	301	-	5,5,5	0.08	0	5,5,5	0.24	0
3	GOL	A	302	-	5,5,5	0.13	0	5,5,5	0.38	0
3	GOL	B	301	-	5,5,5	0.19	0	5,5,5	0.40	0

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	GOL	A	301	-	-	0/4/4/4	-
3	GOL	A	302	-	-	2/4/4/4	-
3	GOL	B	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	GOL	C1-C2-C3-O3
3	B	301	GOL	O1-C1-C2-C3
3	B	301	GOL	O2-C2-C3-O3
3	A	302	GOL	O2-C2-C3-O3
3	B	301	GOL	O1-C1-C2-O2
3	B	301	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.









5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.49	12 (9%)  	50, 64, 112, 162	0
1	B	133/139 (95%)	0.64	17 (12%)  	54, 70, 120, 148	0
2	C	261/275 (94%)	0.27	14 (5%)  	47, 64, 103, 133	0
All	All	518/553 (93%)	0.42	43 (8%)  	47, 66, 110, 162	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	216	VAL	9.6
2	C	83	GLN	8.8
1	A	216	VAL	6.7
1	A	162	THR	5.8
1	A	163	ASN	5.2
1	A	215	THR	4.9
1	B	164	GLY	4.8
1	A	161	PRO	4.7
1	A	190	ALA	3.9
2	C	274	SER	3.6
1	B	163	ASN	3.4
2	C	84	LYS	3.4
1	B	155	MET	3.4
2	C	42	ARG	3.3
1	B	85	GLN	3.2
1	A	214	ARG	3.0
1	B	161	PRO	3.0
1	B	215	THR	2.9
1	A	164	GLY	2.9
1	A	155	MET	2.8
1	A	191	LEU	2.8
1	B	135	LEU	2.8
1	B	173	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	60	ASP	2.6
1	B	162	THR	2.6
1	B	104	ILE	2.5
1	B	101	LYS	2.5
1	A	101	LYS	2.5
2	C	1	GLU	2.4
2	C	44	LYS	2.4
2	C	123	GLU	2.3
2	C	251	GLN	2.3
2	C	195	GLU	2.2
1	B	156	GLY	2.2
1	B	171	GLY	2.2
1	B	95	TYR	2.1
1	A	134	LEU	2.1
2	C	58	THR	2.1
2	C	273	PRO	2.1
1	B	186	LYS	2.0
1	B	108	ASN	2.0
2	C	131	GLN	2.0
2	C	179	ARG	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 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(Å ²)	Q<0.9
3	GOL	B	301	6/6	0.60	0.28	79,101,104,105	0
3	GOL	A	302	6/6	0.72	0.46	80,96,100,108	0
3	GOL	A	301	6/6	0.90	0.27	89,95,98,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.