



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2021 – 12:07 PM JST

PDB ID : 7DHA
Title : crystal structure of CD38 in complex with daratumumab
Authors : Lee, H.T.; Heo, Y.S.
Deposited on : 2020-11-13
Resolution : 2.55 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 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	:	2.23.1
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)	:	2.23.1

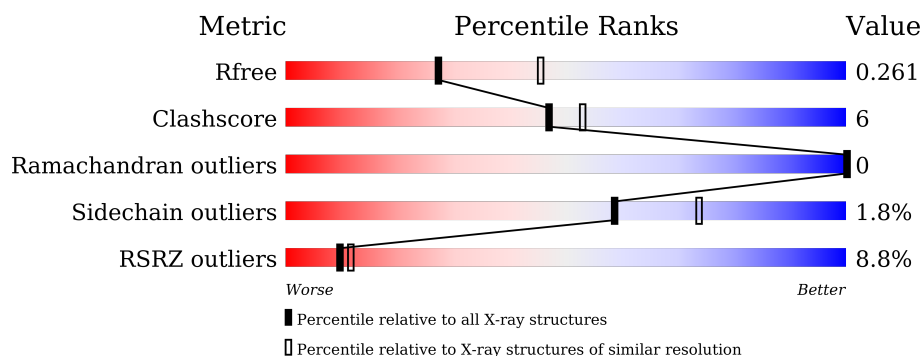
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	265	<div> <div>11%</div> <div>74%</div> <div>20%</div> <div>6%</div> </div>
2	B	214	<div> <div>7%</div> <div>86%</div> <div>13%</div> <div>•</div> </div>
3	C	234	<div> <div>7%</div> <div>83%</div> <div>11%</div> <div>• 5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5425 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 ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			2001	1263	342	380	16			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	ASP	ASN	engineered mutation	UNP P28907
A	120	ALA	ASN	engineered mutation	UNP P28907
A	165	ASP	ASN	engineered mutation	UNP P28907
A	175	ASP	ASN	engineered mutation	UNP P28907
A	257	GLY	-	expression tag	UNP P28907
A	258	THR	-	expression tag	UNP P28907
A	259	LYS	-	expression tag	UNP P28907
A	260	HIS	-	expression tag	UNP P28907
A	261	HIS	-	expression tag	UNP P28907
A	262	HIS	-	expression tag	UNP P28907
A	263	HIS	-	expression tag	UNP P28907
A	264	HIS	-	expression tag	UNP P28907
A	265	HIS	-	expression tag	UNP P28907

- Molecule 2 is a protein called Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1631	1021	278	328	4			

- Molecule 3 is a protein called Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	222	Total	C	N	O	S	0	0	0
			1650	1048	273	323	6			

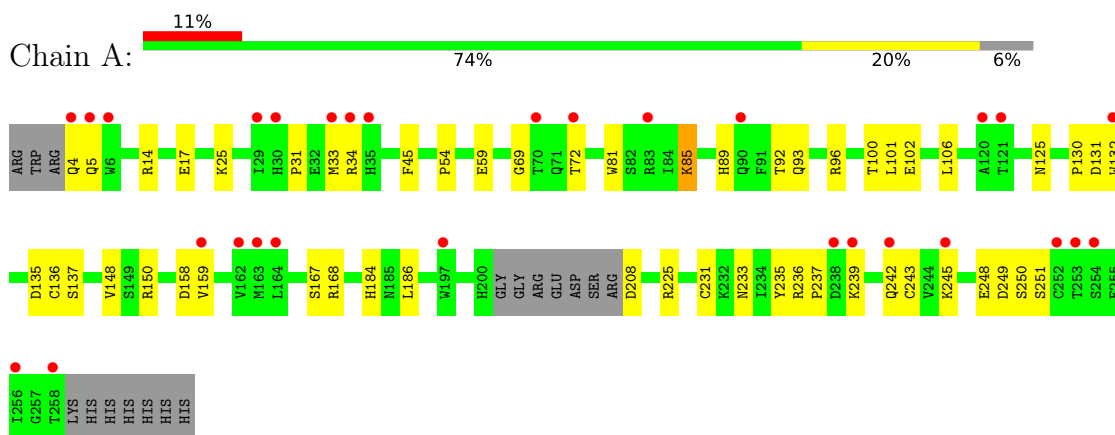
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total 55	O 55	0	0
4	B	34	Total 34	O 34	0	0
4	C	54	Total 54	O 54	0	0

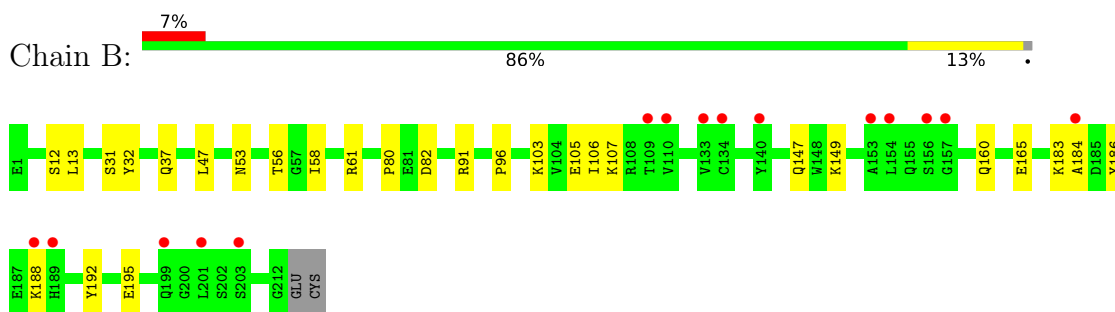
3 Residue-property plots [i](#)

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.

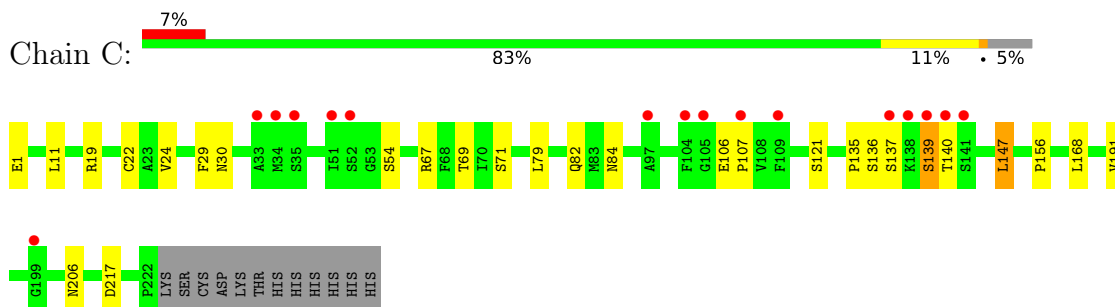
- Molecule 1: ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase 1



- Molecule 2: Light chain



- Molecule 3: Heavy Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	80.24Å 54.16Å 92.69Å 90.00° 98.88° 90.00°	Depositor
Resolution (Å)	29.09 – 2.55 29.09 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.09-2.55) 98.0 (29.09-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.207 , 0.261 0.207 , 0.261	Depositor DCC
R_{free} test set	2000 reflections (7.84%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5425	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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

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	0.30	0/2049	0.48	1/2777 (0.0%)
2	B	0.28	0/1668	0.49	0/2269
3	C	0.29	0/1691	0.51	0/2302
All	All	0.29	0/5408	0.49	1/7348 (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	34	ARG	NE-CZ-NH1	6.43	123.52	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	PRO	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	2001	0	1935	32	0
2	B	1631	0	1587	20	0
3	C	1650	0	1618	16	0
4	A	55	0	0	3	1
4	B	34	0	0	6	1
4	C	54	0	0	3	0
All	All	5425	0	5140	65	1

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 6.

All (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLY:HA3	1:A:106:LEU:HD11	1.49	0.94
2:B:160:GLN:NE2	4:B:302:HOH:O	2.04	0.89
2:B:53:ASN:OD1	4:B:301:HOH:O	2.00	0.78
1:A:242:GLN:HA	1:A:245:LYS:HD2	1.67	0.75
1:A:33:MET:HG3	1:A:72:THR:H	1.50	0.74
3:C:135:PRO:HG3	3:C:147:LEU:HB3	1.70	0.74
2:B:165:GLU:OE2	4:B:303:HOH:O	2.06	0.73
1:A:243:CYS:SG	1:A:251:SER:OG	2.43	0.72
3:C:1:GLU:O	4:C:301:HOH:O	2.10	0.69
1:A:186:LEU:O	1:A:225:ARG:NH2	2.27	0.68
3:C:168:LEU:HD21	3:C:191:VAL:HG21	1.75	0.67
2:B:82:ASP:OD1	4:B:304:HOH:O	2.11	0.67
1:A:236:ARG:HB3	1:A:239:LYS:HB3	1.77	0.66
3:C:206:ASN:ND2	3:C:217:ASP:OD1	2.26	0.66
3:C:71:SER:OG	4:C:302:HOH:O	2.13	0.65
3:C:106:GLU:OE2	4:C:303:HOH:O	2.14	0.65
1:A:208:ASP:OD1	1:A:233:ASN:ND2	2.29	0.64
1:A:248:GLU:HG3	2:B:56:THR:HG23	1.80	0.64
1:A:131:ASP:N	1:A:135:ASP:OD2	2.31	0.61
1:A:25:LYS:NZ	4:A:302:HOH:O	2.22	0.61
2:B:80:PRO:HA	2:B:106:ILE:HG12	1.83	0.60
2:B:32:TYR:HB3	2:B:91:ARG:HG3	1.83	0.60
1:A:132:TRP:HD1	1:A:137:SER:HA	1.66	0.60
1:A:33:MET:N	1:A:33:MET:SD	2.76	0.59
3:C:11:LEU:HB2	3:C:156:PRO:HG3	1.86	0.57
1:A:136:CYS:HB2	4:A:330:HOH:O	2.08	0.53
2:B:103:LYS:NZ	2:B:105:GLU:OE1	2.41	0.53
1:A:92:THR:HG21	1:A:100:THR:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:LYS:HE3	2:B:195:GLU:HG3	1.91	0.52
1:A:132:TRP:CD1	1:A:137:SER:HA	2.45	0.52
1:A:14:ARG:HH21	1:A:17:GLU:HG2	1.75	0.52
2:B:13:LEU:O	2:B:107:LYS:N	2.37	0.52
3:C:24:VAL:HG21	3:C:29:PHE:CD1	2.46	0.51
1:A:54:PRO:HB2	1:A:130:PRO:HG2	1.93	0.50
1:A:251:SER:N	4:A:305:HOH:O	2.39	0.50
2:B:96:PRO:HG3	3:C:107:PRO:HD2	1.94	0.49
1:A:249:ASP:OD1	1:A:250:SER:N	2.46	0.48
2:B:147:GLN:HB3	2:B:195:GLU:HB2	1.96	0.47
3:C:136:SER:OG	3:C:137:SER:N	2.49	0.46
3:C:22:CYS:HB3	3:C:79:LEU:HB3	1.97	0.45
1:A:4:GLN:O	1:A:130:PRO:HG3	2.17	0.45
2:B:61:ARG:NH2	2:B:82:ASP:OD2	2.50	0.45
3:C:67:ARG:HB3	3:C:84:ASN:O	2.17	0.45
2:B:186:TYR:O	2:B:192:TYR:OH	2.29	0.45
1:A:81:TRP:CZ3	1:A:85:LYS:HG3	2.52	0.44
3:C:139:SER:O	3:C:140:THR:OG1	2.30	0.44
1:A:158:ASP:O	1:A:159:VAL:HG23	2.17	0.44
3:C:11:LEU:HD11	3:C:121:SER:HB3	2.00	0.44
1:A:14:ARG:HE	1:A:14:ARG:HB3	1.66	0.44
1:A:59:GLU:OE2	1:A:150:ARG:NH1	2.51	0.43
2:B:47:LEU:HD23	2:B:58:ILE:HD12	1.99	0.43
1:A:89:HIS:NE2	1:A:102:GLU:HB2	2.34	0.42
1:A:101:LEU:HD21	1:A:148:VAL:HG13	2.01	0.42
1:A:69:GLY:HA3	1:A:106:LEU:CD1	2.35	0.42
1:A:89:HIS:O	1:A:93:GLN:HG2	2.19	0.42
1:A:5:GLN:OE1	1:A:125:ASN:ND2	2.41	0.42
2:B:37:GLN:HB2	2:B:47:LEU:HD11	2.02	0.41
2:B:184:ALA:O	2:B:188:LYS:HG3	2.20	0.41
1:A:4:GLN:HG3	1:A:5:GLN:H	1.85	0.41
1:A:231:CYS:O	3:C:54:SER:HB3	2.20	0.41
2:B:53:ASN:N	4:B:301:HOH:O	2.53	0.41
2:B:183:LYS:NZ	4:B:307:HOH:O	2.41	0.41
3:C:69:THR:HB	3:C:82:GLN:HB3	2.02	0.41
2:B:12:SER:HA	2:B:105:GLU:O	2.22	0.40
1:A:235:TYR:O	1:A:237:PRO:HD3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:329:HOH:O	4:B:329:HOH:O[2_656]	2.15	0.05

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	244/265 (92%)	231 (95%)	13 (5%)	0	100	100
2	B	210/214 (98%)	202 (96%)	8 (4%)	0	100	100
3	C	220/234 (94%)	214 (97%)	6 (3%)	0	100	100
All	All	674/713 (94%)	647 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	229/244 (94%)	223 (97%)	6 (3%)	46	61
2	B	184/186 (99%)	183 (100%)	1 (0%)	88	93
3	C	184/196 (94%)	180 (98%)	4 (2%)	52	66
All	All	597/626 (95%)	586 (98%)	11 (2%)	59	74

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	PHE
1	A	85	LYS
1	A	96	ARG
1	A	167	SER
1	A	168	ARG
1	A	184	HIS
2	B	31	SER
3	C	19	ARG
3	C	30	ASN
3	C	139	SER
3	C	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
1	A	246	ASN
2	B	166	GLN

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

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	248/265 (93%)	0.66	29 (11%) 4 6	32, 50, 79, 107	0
2	B	212/214 (99%)	0.43	15 (7%) 16 19	30, 54, 80, 94	0
3	C	222/234 (94%)	0.28	16 (7%) 15 18	28, 39, 61, 124	0
All	All	682/713 (95%)	0.47	60 (8%) 10 11	28, 47, 79, 124	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	139	SER	7.7
1	A	34	ARG	6.8
3	C	138	LYS	6.4
3	C	140	THR	5.5
2	B	201	LEU	4.5
1	A	4	GLN	4.4
2	B	109	THR	4.3
1	A	162	VAL	3.9
1	A	5	GLN	3.8
2	B	184	ALA	3.5
2	B	110	VAL	3.4
3	C	137	SER	3.3
1	A	258	THR	3.3
3	C	141	SER	3.2
1	A	120	ALA	3.2
2	B	203	SER	3.2
3	C	33	ALA	3.1
1	A	29	ILE	3.1
2	B	199	GLN	3.0
1	A	242	GLN	2.9
1	A	256	ILE	2.9
1	A	72	THR	2.9
1	A	239	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	154	LEU	2.8
1	A	159	VAL	2.7
3	C	105	GLY	2.7
2	B	156	SER	2.7
2	B	188	LYS	2.7
1	A	252	CYS	2.6
2	B	140	TYR	2.6
1	A	90	GLN	2.6
3	C	107	PRO	2.6
1	A	33	MET	2.6
3	C	51	ILE	2.5
1	A	70	THR	2.5
1	A	245	LYS	2.5
3	C	97	ALA	2.5
2	B	189	HIS	2.4
1	A	121	THR	2.4
2	B	157	GLY	2.4
1	A	197	TRP	2.4
3	C	35	SER	2.4
1	A	6	TRP	2.3
1	A	253	THR	2.3
3	C	199	GLY	2.3
1	A	132	TRP	2.2
2	B	153	ALA	2.2
3	C	109	PHE	2.2
1	A	35	HIS	2.2
1	A	30	HIS	2.2
1	A	164	LEU	2.2
1	A	163	MET	2.1
2	B	133	VAL	2.1
3	C	104	PHE	2.1
1	A	238	ASP	2.1
3	C	34	MET	2.1
1	A	83	ARG	2.1
2	B	134	CYS	2.1
1	A	254	SER	2.0
3	C	52	SER	2.0

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 [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.