



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:54 AM GMT

PDB ID : 3K51
Title : Crystal Structure of DcR3-TL1A complex
Authors : Zhan, C.; Patskovsky, Y.; Yan, Q.; Li, Z.; Ramagopal, U.A.; Nathenson, S.G.; Almo, S.C.
Deposited on : 2009-10-06
Resolution : 2.45 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

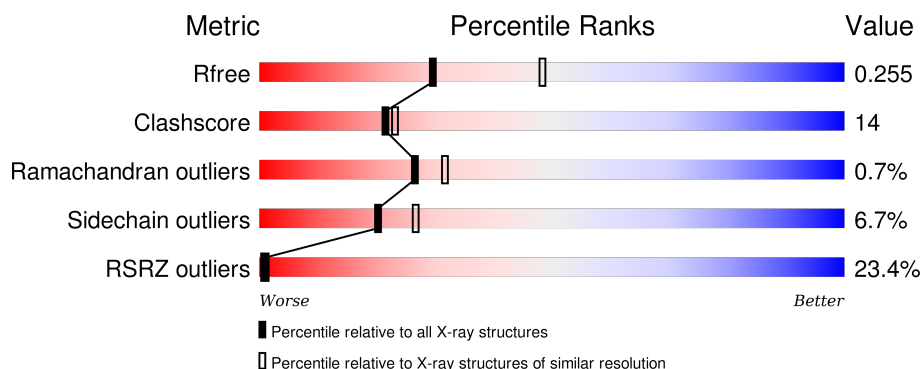
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

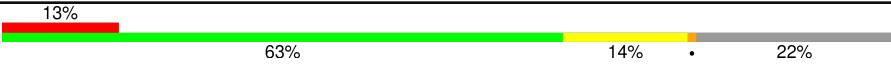

The reported resolution of this entry is 2.45 Å.

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}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	184	
2	B	176	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2456 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 Tumor necrosis factor ligand superfamily member 15, secreted form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	5	0
			1154	750	185	214	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP O95150
A	2	SER	-	EXPRESSION TAG	UNP O95150
A	3	HIS	-	EXPRESSION TAG	UNP O95150
A	4	MET	-	EXPRESSION TAG	UNP O95150
A	95	SER	CYS	ENGINEERED	UNP O95150
A	135	SER	CYS	ENGINEERED	UNP O95150

- Molecule 2 is a protein called Decoy receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	161	Total	C	N	O	S	0	1	0
			1219	740	233	228	18			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ARG	-	EXPRESSION TAG	UNP O95407
B	29	SER	-	EXPRESSION TAG	UNP O95407
B	196	THR	-	EXPRESSION TAG	UNP O95407
B	197	GLY	-	EXPRESSION TAG	UNP O95407
B	198	HIS	-	EXPRESSION TAG	UNP O95407
B	199	HIS	-	EXPRESSION TAG	UNP O95407
B	200	HIS	-	EXPRESSION TAG	UNP O95407
B	201	HIS	-	EXPRESSION TAG	UNP O95407
B	202	HIS	-	EXPRESSION TAG	UNP O95407

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Chain	Residue	Modelled	Actual	Comment	Reference
B	203	HIS	-	EXPRESSION TAG	UNP O95407

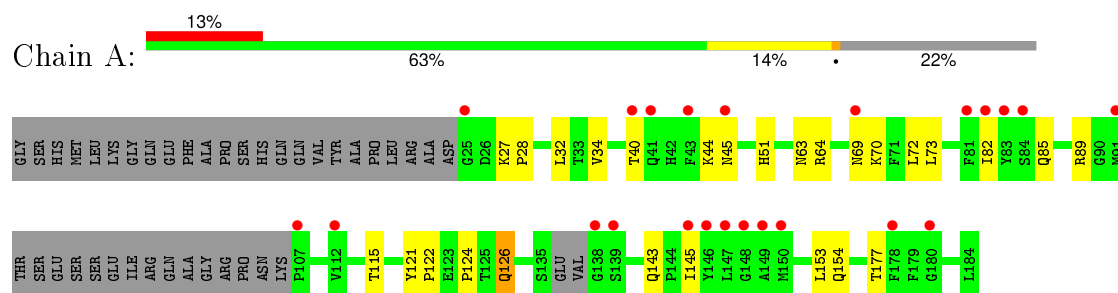
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	57	Total O 57 57	0	0
3	B	26	Total O 26 26	0	0

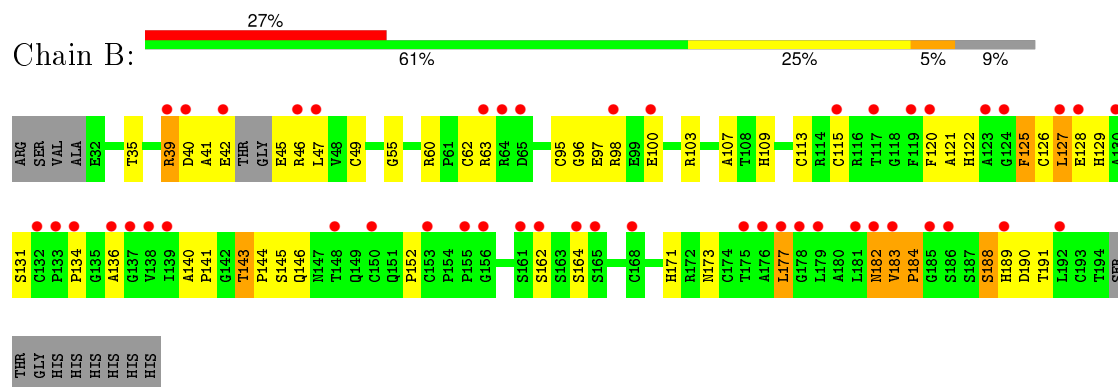
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Tumor necrosis factor ligand superfamily member 15, secreted form



- Molecule 2: Decoy receptor 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	74.89Å 74.89Å 143.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.23 – 2.45 36.23 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.23-2.45) 99.9 (36.23-2.45)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.223 , 0.262 0.222 , 0.255	Depositor DCC
R_{free} test set	562 reflections (3.27%)	DCC
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.5	EDS
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 17777 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2456	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.37	0/1197	0.45	0/1621
2	B	0.31	0/1259	0.48	1/1718 (0.1%)
All	All	0.34	0/2456	0.46	1/3339 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	183	VAL	C-N-CD	-7.63	103.81	120.60

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	1154	0	1137	18	0
2	B	1219	0	1101	45	0
3	A	57	0	0	1	0
3	B	26	0	0	0	0
All	All	2456	0	2238	63	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 14.

All (63) 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:B:49:CYS:CB	2:B:62:CYS:SG	2.29	1.21
2:B:127:LEU:HD23	2:B:127:LEU:H	1.13	1.13
2:B:127:LEU:CD2	2:B:127:LEU:H	1.65	1.09
2:B:96:GLY:O	2:B:97:GLU:HG2	1.54	1.06
2:B:95:CYS:SG	2:B:113:CYS:CB	2.44	1.05
2:B:49:CYS:SG	2:B:62:CYS:CB	2.49	1.00
2:B:97:GLU:HG3	2:B:98:ARG:H	1.26	0.97
2:B:127:LEU:CD2	2:B:127:LEU:N	2.30	0.87
2:B:127:LEU:HD23	2:B:127:LEU:N	1.89	0.85
2:B:97:GLU:CG	2:B:98:ARG:H	1.91	0.80
1:A:69:ASN:O	1:A:70:LYS:HB2	1.79	0.79
2:B:39:ARG:HD2	2:B:39:ARG:H	1.49	0.77
2:B:182:ASN:OD1	2:B:183:VAL:N	2.20	0.75
2:B:97:GLU:HG3	2:B:98:ARG:N	2.01	0.74
2:B:97:GLU:CG	2:B:98:ARG:N	2.50	0.71
2:B:115:CYS:SG	2:B:121:ALA:HB2	2.31	0.71
1:A:51:HIS:CE1	1:A:70:LYS:HE3	2.25	0.70
2:B:182:ASN:OD1	2:B:182:ASN:C	2.30	0.69
1:A:69:ASN:O	1:A:70:LYS:CB	2.41	0.69
2:B:95:CYS:CB	2:B:113:CYS:SG	2.80	0.67
2:B:127:LEU:HD22	2:B:127:LEU:N	2.09	0.63
2:B:39:ARG:N	2:B:39:ARG:HD2	2.14	0.63
2:B:127:LEU:HD22	2:B:127:LEU:H	1.59	0.62
2:B:188:SER:O	2:B:189:HIS:HB2	2.00	0.61
1:A:51:HIS:CE1	1:A:70:LYS:CE	2.83	0.61
1:A:32:LEU:HD11	1:A:72:LEU:HD13	1.85	0.59
1:A:82[A]:ILE:HD11	1:A:153:LEU:HD11	1.87	0.57
1:A:63:ASN:O	1:A:64:ARG:HB2	2.07	0.53
1:A:89[A]:ARG:HH21	1:A:89[A]:ARG:HG3	1.73	0.53
2:B:120:PHE:O	2:B:127:LEU:HD23	2.09	0.52
2:B:143:THR:C	2:B:145:SER:H	2.14	0.51
2:B:173:ASN:O	2:B:177:LEU:HB2	2.11	0.51
2:B:96:GLY:O	2:B:97:GLU:CG	2.44	0.51
1:A:44:LYS:O	1:A:45:ASN:CB	2.60	0.50
2:B:49:CYS:CA	2:B:62:CYS:SG	2.98	0.50
2:B:143:THR:O	2:B:145:SER:N	2.45	0.50
2:B:125:PHE:HD2	2:B:126:CYS:H	1.60	0.50
2:B:188:SER:O	2:B:189:HIS:CB	2.60	0.50
2:B:40:ASP:OD1	2:B:41:ALA:N	2.45	0.49
2:B:171:HIS:HD2	2:B:190:ASP:HA	1.78	0.49
2:B:143:THR:HG23	2:B:146:GLN:H	1.77	0.48
2:B:184:PRO:HA	2:B:191:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:CYS:SG	2:B:113:CYS:HB3	2.48	0.46
2:B:60:ARG:HH21	2:B:63:ARG:HD2	1.82	0.45
1:A:126[A]:GLN:NE2	3:A:226:HOH:O	2.44	0.44
2:B:143:THR:C	2:B:145:SER:N	2.70	0.44
1:A:115:THR:CG2	1:A:124:PRO:HB2	2.48	0.44
2:B:55:GLY:HA2	2:B:107:ALA:O	2.18	0.43
2:B:136:ALA:HA	2:B:152:PRO:HA	1.99	0.43
2:B:131:SER:HA	2:B:164:SER:HB3	2.00	0.43
1:A:89[A]:ARG:HG3	1:A:89[A]:ARG:NH2	2.33	0.43
1:A:51:HIS:CE1	1:A:70:LYS:HE2	2.53	0.43
2:B:42:GLU:HG2	2:B:45:GLU:OE2	2.18	0.42
1:A:72:LEU:HD12	1:A:72:LEU:HA	1.92	0.42
2:B:134:PRO:HD3	2:B:162:SER:HB3	2.02	0.41
2:B:171:HIS:HA	2:B:190:ASP:OD1	2.20	0.41
2:B:128:GLU:HG3	2:B:129:HIS:N	2.35	0.41
2:B:103:ARG:NH1	2:B:109:HIS:CE1	2.89	0.41
1:A:85:GLN:HA	1:A:145:ILE:O	2.20	0.41
2:B:140:ALA:HA	2:B:141:PRO:HD2	1.90	0.40
1:A:27:LYS:HA	1:A:28:PRO:HD3	1.94	0.40
1:A:34:VAL:HB	1:A:177:THR:HB	2.04	0.40
1:A:121:TYR:HA	1:A:122:PRO:HD3	1.85	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	142/184 (77%)	137 (96%)	5 (4%)	0	100	100
2	B	158/176 (90%)	147 (93%)	9 (6%)	2 (1%)	15	15
All	All	300/360 (83%)	284 (95%)	14 (5%)	2 (1%)	26	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	184	PRO
2	B	144	PRO

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	128/163 (78%)	122 (95%)	6 (5%)	32	45
2	B	132/148 (89%)	120 (91%)	12 (9%)	12	13
All	All	260/311 (84%)	242 (93%)	18 (7%)	20	25

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	73	LEU
1	A	126[A]	GLN
1	A	126[B]	GLN
1	A	143	GLN
1	A	154	GLN
2	B	35	THR
2	B	39	ARG
2	B	46	ARG
2	B	47	LEU
2	B	100	GLU
2	B	122	HIS
2	B	125	PHE
2	B	127	LEU
2	B	143	THR
2	B	177	LEU
2	B	182	ASN
2	B	188	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	63	ASN
2	B	109	HIS
2	B	171	HIS
2	B	189	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 carbohydrates 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 [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, 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	143/184 (77%)	0.81	23 (16%)	3 2	37, 52, 99, 122	0
2	B	161/176 (91%)	1.23	48 (29%)	1 0	44, 114, 153, 163	0
All	All	304/360 (84%)	1.03	71 (23%)	1 1	37, 65, 148, 163	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	GLY	7.0
1	A	41	GLN	6.4
2	B	98	ARG	5.9
2	B	148	THR	5.3
1	A	25	GLY	5.3
1	A	45	ASN	5.3
2	B	189	HIS	4.9
2	B	46	ARG	4.9
2	B	117	THR	4.7
2	B	176	ALA	4.6
2	B	168	CYS	4.6
2	B	127	LEU	4.4
1	A	43	PHE	4.4
1	A	40	THR	4.4
1	A	148	GLY	4.1
2	B	161	SER	4.0
2	B	162	SER	4.0
1	A	149	ALA	3.8
2	B	182	ASN	3.8
1	A	146	TYR	3.7
2	B	165	SER	3.7
2	B	123	ALA	3.7
2	B	39	ARG	3.7
1	A	147	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	119	PHE	3.3
1	A	83	TYR	3.2
2	B	156	GLY	3.2
2	B	40	ASP	3.2
2	B	175	THR	3.2
1	A	81	PHE	3.1
2	B	150	CYS	3.0
2	B	177	LEU	2.9
2	B	132	CYS	2.9
2	B	64	ARG	2.9
1	A	139	SER	2.8
2	B	192	LEU	2.8
2	B	120	PHE	2.8
2	B	134	PRO	2.7
2	B	179	LEU	2.7
2	B	65	ASP	2.7
1	A	82[A]	ILE	2.7
2	B	42	GLU	2.7
2	B	136	ALA	2.6
1	A	145	ILE	2.6
2	B	139	ILE	2.6
2	B	137	GLY	2.6
2	B	47	LEU	2.6
2	B	133	PRO	2.6
1	A	84	SER	2.6
1	A	180	GLY	2.6
2	B	155	PRO	2.6
1	A	91	MET	2.5
2	B	124	GLY	2.5
2	B	153	CYS	2.5
2	B	185	GLY	2.5
2	B	138	VAL	2.5
2	B	178	GLY	2.5
2	B	100	GLU	2.5
2	B	130	ALA	2.4
2	B	128	GLU	2.4
2	B	63	ARG	2.4
2	B	164	SER	2.3
1	A	69	ASN	2.3
2	B	186	SER	2.3
1	A	112	VAL	2.3
1	A	150	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	178	PHE	2.2
2	B	183	VAL	2.2
2	B	115	CYS	2.2
2	B	181	LEU	2.2
1	A	107	PRO	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 carbohydrates 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.