WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 04:12 PM JST

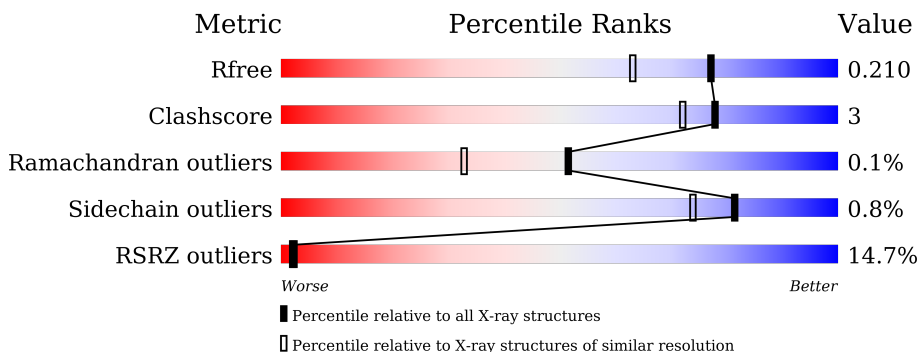|		
PDB ID	:	8JEP
Title	:	Crystal structure of Ociperlimab
Authors	:	Sun, J.; Zhang, X.X.; Song, J.
Deposited on	:	2023-05-16
Resolution	:	1.70 Å(reported)

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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 1.70 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	Percentile Ranks	Value
Rfree		0.210
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		0.8%
RSRZ outliers		14.7%

Worse ◼ ◼ Better

◼ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	228	16% / 86% 9% 5%
1	C	228	15% / 89% 6% 6%
2	B	214	10% / 94% 5%
2	D	214	15% / 95% 5%

WORLDWIDE wwPDB PROTEIN DATA BANK

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7344 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 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total 1640	C 1040	N 270	O 322	S 8	0	0	0
1	C	215	Total 1630	C 1035	N 268	O 319	S 8	0	0	0

- Molecule 2 is a protein called antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total 1638	C 1027	N 275	O 330	S 6	0	0	0
2	D	214	Total 1638	C 1027	N 275	O 330	S 6	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	213	Total 213	O 213	0	0
3	B	222	Total 222	O 222	0	0
3	C	195	Total 195	O 195	0	0
3	D	168	Total 168	O 168	0	0

3 Residue-property plots ⓘ

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.
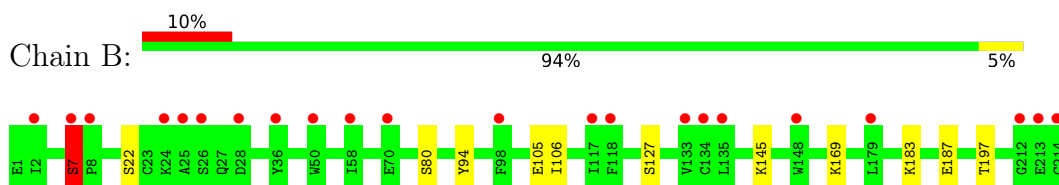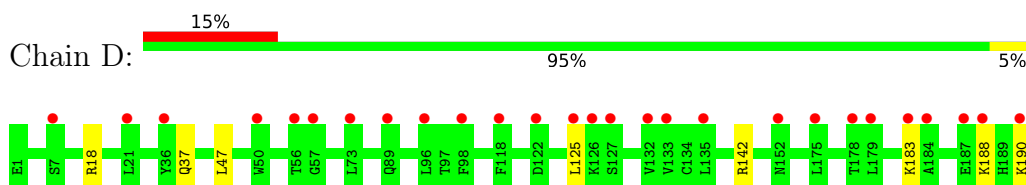
- Molecule 1: antibody heavy chain
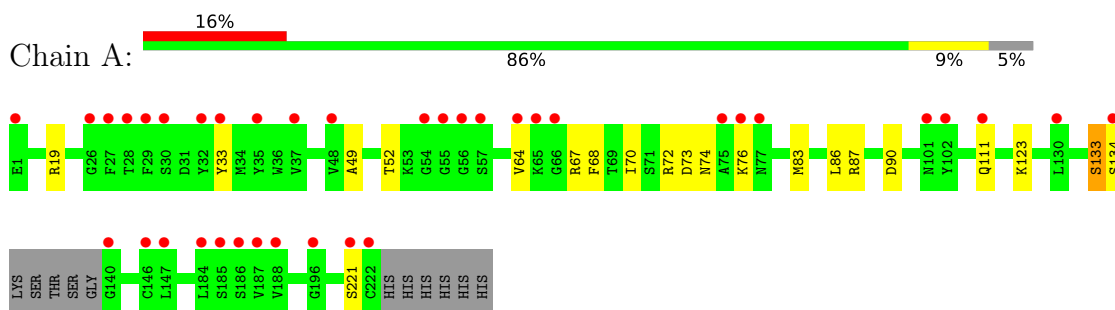
Chain A:

- Molecule 1: antibody heavy chain

Chain C:
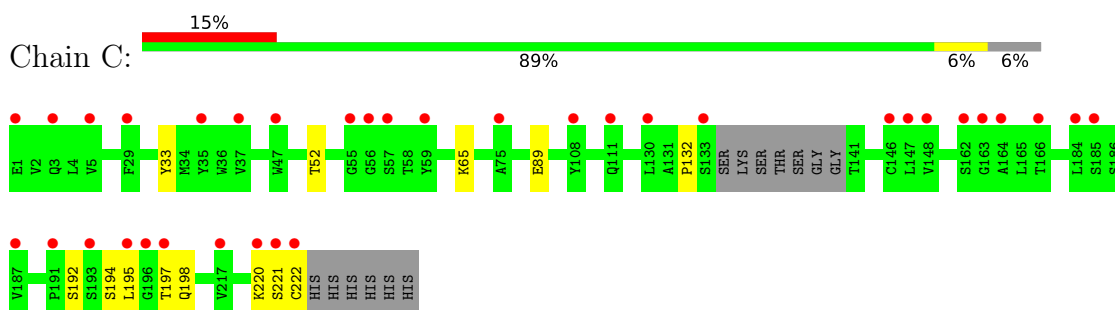
- Molecule 2: antibody light chain

Chain B:

- Molecule 2: antibody light chain

Chain D:

R211 G212 E213 C214

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.50Å 112.30Å 159.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.86 – 1.70 26.65 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.86-1.70) 100.0 (26.65-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.184 , 0.210 0.184 , 0.210	Depositor DCC
R_{free} test set	6293 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7344	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.35	0/1681	0.56	0/2290
1	C	0.33	0/1671	0.56	0/2277
2	B	0.37	0/1675	0.57	0/2276
2	D	0.34	0/1675	0.54	0/2276
All	All	0.35	0/6702	0.56	0/9119

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	1640	0	1591	15	0
1	C	1630	0	1583	8	0
2	B	1638	0	1588	8	0
2	D	1638	0	1588	7	0
3	A	213	0	0	4	2
3	B	222	0	0	2	2
3	C	195	0	0	3	2
3	D	168	0	0	1	0
All	All	7344	0	6350	37	3

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 3.

All (37) 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:C:65:LYS:NZ	3:C:301:HOH:O	2.02	0.91
1:A:111:GLN:NE2	3:A:301:HOH:O	2.16	0.79
1:C:132:PRO:O	3:C:302:HOH:O	2.04	0.75
1:A:67:ARG:NH1	1:A:90:ASP:OD2	2.21	0.73
1:A:72:ARG:HE	1:A:74:ASN:HD21	1.39	0.70
1:C:89:GLU:HG3	3:C:398:HOH:O	1.93	0.69
2:D:195:GLU:OE1	3:D:301:HOH:O	2.10	0.69
1:A:133:SER:OG	1:A:134:SER:N	2.26	0.69
2:B:7:SER:HB3	2:B:22:SER:HB2	1.75	0.68
1:A:83:MET:HE2	1:A:86:LEU:HD21	1.75	0.68
1:C:220:LYS:HG2	1:C:221:SER:H	1.64	0.63
1:C:194:SER:HA	1:C:197:THR:HG22	1.82	0.61
2:D:125:LEU:HD22	2:D:183:LYS:HG3	1.82	0.60
1:A:72:ARG:NE	1:A:74:ASN:HD21	2.02	0.57
1:A:19:ARG:NH2	3:A:302:HOH:O	2.19	0.56
1:C:192:SER:HA	1:C:195:LEU:HD13	1.87	0.55
2:B:169:LYS:O	2:D:18:ARG:NH1	2.37	0.54
2:B:127:SER:HB3	3:B:411:HOH:O	2.06	0.53
2:B:94:TYR:O	3:B:302:HOH:O	2.19	0.53
1:A:64:VAL:HG13	1:A:68:PHE:CG	2.44	0.52
2:D:125:LEU:O	2:D:183:LYS:HD3	2.11	0.51
2:D:191:VAL:HG22	2:D:210:ASN:ND2	2.25	0.51
1:C:33:TYR:CD2	1:C:52:THR:HA	2.49	0.48
1:A:87:ARG:NH1	3:A:309:HOH:O	2.45	0.47
1:A:123:LYS:HE3	3:A:399:HOH:O	2.15	0.46
1:C:194:SER:HB2	1:C:198:GLN:HB3	1.98	0.46
1:A:49:ALA:HB1	1:A:70:ILE:HB	1.98	0.45
1:A:33:TYR:CD2	1:A:52:THR:HA	2.51	0.45
2:B:105:GLU:HG2	2:B:106:ILE:N	2.33	0.44
2:D:188:LYS:HB3	2:D:188:LYS:HE2	1.84	0.44
2:B:183:LYS:O	2:B:187:GLU:HG3	2.18	0.43
2:D:37:GLN:HB2	2:D:47:LEU:HD11	2.01	0.42
2:B:80:SER:HA	2:B:106:ILE:HG12	2.02	0.42
1:A:72:ARG:HE	1:A:74:ASN:ND2	2.10	0.42
1:A:73:ASP:OD1	1:A:76:LYS:HD2	2.20	0.41
1:A:134:SER:O	1:A:134:SER:OG	2.23	0.41
2:B:145:LYS:HB3	2:B:197:THR:HB	2.03	0.40

All (3) 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)
3:A:470:HOH:O	3:C:461:HOH:O[3_546]	1.83	0.37
3:B:441:HOH:O	3:C:462:HOH:O[3_556]	1.98	0.22
3:A:462:HOH:O	3:B:437:HOH:O[4_566]	1.99	0.21

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	213/228 (93%)	209 (98%)	4 (2%)	0	100	100
1	C	211/228 (92%)	208 (99%)	3 (1%)	0	100	100
2	B	212/214 (99%)	207 (98%)	4 (2%)	1 (0%)	29	13
2	D	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
All	All	848/884 (96%)	833 (98%)	14 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	7	SER

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	182/192 (95%)	180 (99%)	2 (1%)	73	63
1	C	181/192 (94%)	180 (99%)	1 (1%)	86	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	184/184 (100%)	183 (100%)	1 (0%)	88	83
2	D	184/184 (100%)	182 (99%)	2 (1%)	73	63
All	All	731/752 (97%)	725 (99%)	6 (1%)	81	74

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	SER
1	A	221	SER
2	B	7	SER
1	C	222	CYS
2	D	142	ARG
2	D	190	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
2	D	210	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	217/228 (95%)	0.80	37 (17%)	1	1	24, 41, 70, 86	0
1	C	215/228 (94%)	0.76	35 (16%)	1	1	26, 41, 77, 116	0
2	B	214/214 (100%)	0.53	22 (10%)	6	7	24, 37, 64, 91	0
2	D	214/214 (100%)	0.70	32 (14%)	2	2	29, 42, 65, 108	0
All	All	860/884 (97%)	0.70	126 (14%)	2	2	24, 40, 69, 116	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	221	SER	13.7
1	C	222	CYS	12.9
2	D	214	CYS	11.4
2	B	214	CYS	10.2
1	A	222	CYS	8.3
1	A	221	SER	8.2
1	A	134	SER	7.0
2	B	7	SER	5.8
2	D	212	GLY	5.8
1	A	130	LEU	5.4
1	C	196	GLY	5.2
2	D	50	TRP	5.1
1	A	66	GLY	5.0
1	A	102	TYR	4.9
1	C	164	ALA	4.7
2	B	133	VAL	4.6
1	C	195	LEU	4.6
2	D	133	VAL	4.3
1	A	30	SER	4.3
1	A	65	LYS	4.2
1	C	133	SER	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	135	LEU	4.0
1	A	54	GLY	3.9
2	D	36	TYR	3.9
1	C	130	LEU	3.8
2	D	135	LEU	3.8
2	D	213	GLU	3.8
2	B	212	GLY	3.8
1	A	187	VAL	3.8
2	D	127	SER	3.7
2	D	56	THR	3.6
1	C	29	PHE	3.6
1	A	111	GLN	3.6
2	D	191	VAL	3.5
1	A	1	GLU	3.5
1	A	27	PHE	3.5
1	C	75	ALA	3.5
1	C	108	TYR	3.4
1	C	1	GLU	3.4
1	A	37	VAL	3.3
1	C	191	PRO	3.3
2	D	98	PHE	3.2
2	D	122	ASP	3.2
2	B	118	PHE	3.2
1	A	56	GLY	3.2
1	C	147	LEU	3.2
2	D	125	LEU	3.2
2	D	132	VAL	3.2
2	D	190	LYS	3.2
1	C	35	TYR	3.1
2	B	213	GLU	3.1
1	A	196	GLY	3.1
1	A	147	LEU	3.1
2	B	50	TRP	3.1
1	C	220	LYS	3.0
1	A	29	PHE	3.0
2	D	7	SER	3.0
1	A	140	GLY	3.0
1	A	32	TYR	3.0
1	C	59	TYR	3.0
1	A	184	LEU	3.0
1	C	162	SER	3.0
1	C	47	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	55	GLY	2.9
1	A	64	VAL	2.9
2	D	210	ASN	2.9
1	C	163	GLY	2.9
2	D	118	PHE	2.8
2	D	126	LYS	2.8
2	B	26	SER	2.8
1	A	188	VAL	2.8
1	C	184	LEU	2.8
1	A	146	CYS	2.8
2	D	175	LEU	2.7
1	C	111	GLN	2.7
1	C	56	GLY	2.7
1	C	148	VAL	2.6
1	A	75	ALA	2.6
2	B	98	PHE	2.6
2	B	24	LYS	2.6
1	A	28	THR	2.6
2	B	58	ILE	2.6
2	B	179	LEU	2.6
2	D	184	ALA	2.6
2	D	152	ASN	2.6
2	B	134	CYS	2.6
1	C	166	THR	2.5
2	B	148	TRP	2.5
1	C	37	VAL	2.5
1	A	101	ASN	2.5
1	A	185	SER	2.5
2	B	28	ASP	2.5
2	B	117	ILE	2.5
2	D	21	LEU	2.5
2	D	178	THR	2.4
2	B	25	ALA	2.4
1	C	197	THR	2.4
2	B	70	GLU	2.4
1	C	146	CYS	2.3
1	C	185	SER	2.3
2	B	36	TYR	2.3
2	D	187	GLU	2.3
1	A	33	TYR	2.3
1	C	57	SER	2.3
2	D	57	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	96	LEU	2.3
1	C	193	SER	2.3
1	A	26	GLY	2.3
1	A	77	ASN	2.3
1	C	5	VAL	2.2
1	C	3	GLN	2.2
2	D	89	GLN	2.2
1	A	35	TYR	2.2
1	A	48	VAL	2.2
1	A	57	SER	2.2
2	D	188	LYS	2.2
1	C	187	VAL	2.2
2	B	8	PRO	2.1
2	D	179	LEU	2.1
2	D	183	LYS	2.1
1	C	217	VAL	2.1
2	B	2	ILE	2.1
1	A	186	SER	2.1
1	A	76	LYS	2.0
1	C	55	GLY	2.0
2	D	73	LEU	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.