



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6ISB / pdb_00006isb
Title : crystal structure of human CD226
Authors : Wang, H.; Qi, J.; Zhang, S.; Li, Y.; Tan, S.; Gao, G.F.
Deposited on : 2018-11-16
Resolution : 2.50 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

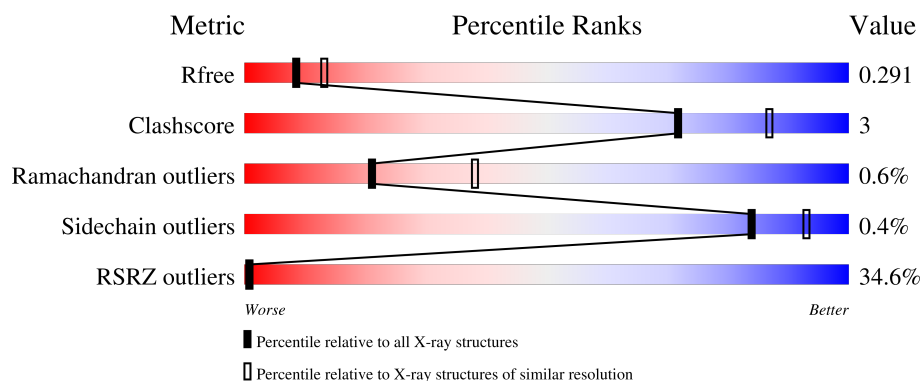
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	232	
1	B	232	
1	C	232	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4354 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.

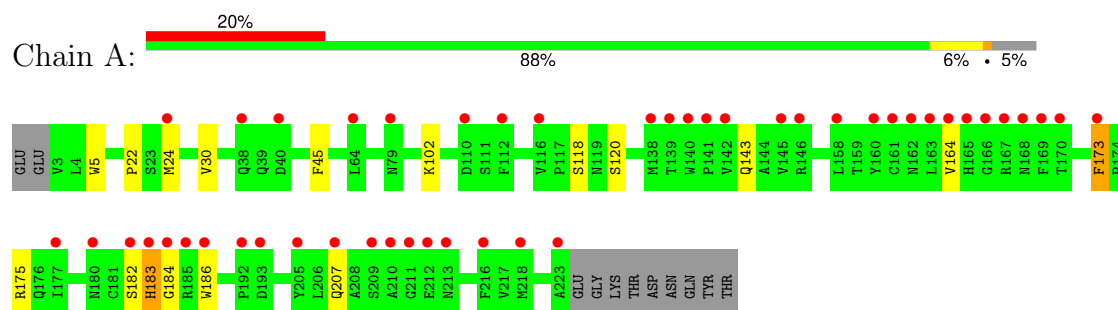
- Molecule 1 is a protein called CD226 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1764	1125	298	328	13			
1	B	218	Total	C	N	O	S	0	0	0
			1739	1111	290	325	13			
1	C	105	Total	C	N	O	S	0	0	0
			851	549	136	160	6			

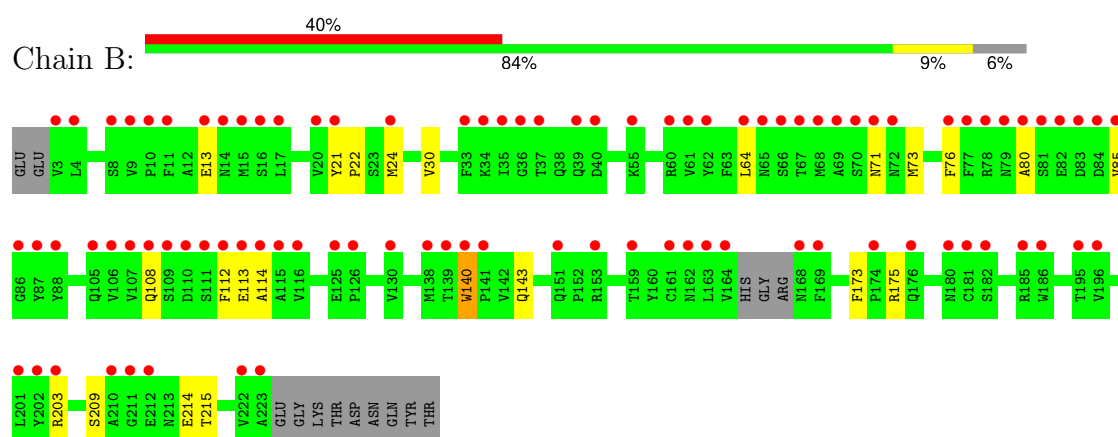
3 Residue-property plots [i](#)

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.

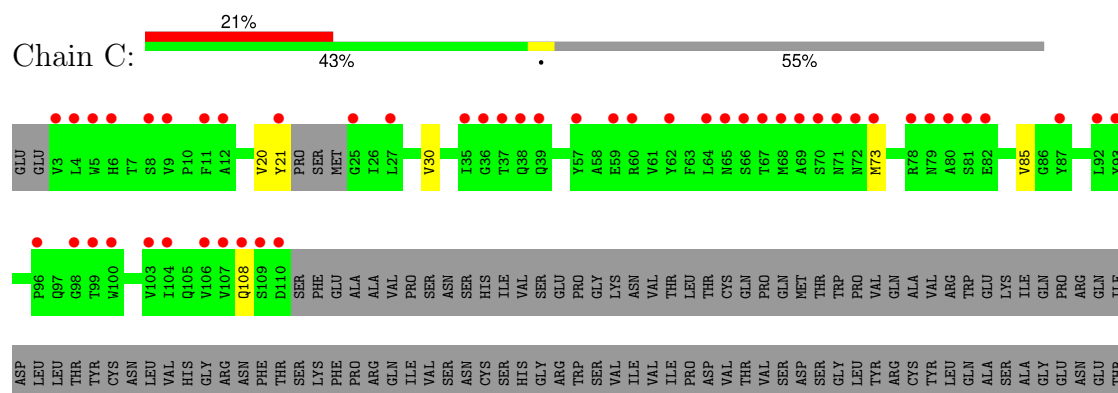
• Molecule 1: CD226 antigen



• Molecule 1: CD226 antigen



• Molecule 1: CD226 antigen



PHE
VAL
MET
ARG
LEU
THR
VAL
ALA
GLU
GLY
LYS
THR
ASP
ASN
GLN
TYR
THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.88Å 118.49Å 123.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.70 – 2.50 42.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.70-2.50) 99.8 (42.70-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.255 , 0.267 0.273 , 0.291	Depositor DCC
R_{free} test set	1504 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4354	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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	0.23	0/1812	0.55	0/2472
1	B	0.25	0/1785	0.52	0/2435
1	C	0.19	0/874	0.50	0/1189
All	All	0.23	0/4471	0.53	0/6096

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	20	VAL	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	1764	0	1708	9	0
1	B	1739	0	1684	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	851	0	809	3	0
All	All	4354	0	4201	28	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 3.

All (28) 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:B:140:TRP:O	1:B:140:TRP:HE3	1.69	0.75
1:A:182:SER:O	1:A:183:HIS:HB2	1.92	0.68
1:B:30:VAL:HG11	1:B:73:MET:HG2	1.82	0.62
1:B:143:GLN:OE1	1:B:209:SER:HA	2.06	0.56
1:B:203:ARG:HD2	1:B:215:THR:HG23	1.89	0.54
1:B:140:TRP:O	1:B:140:TRP:CE3	2.58	0.52
1:B:140:TRP:CH2	1:B:214:GLU:HG3	2.44	0.52
1:A:22:PRO:HG3	1:A:173:PHE:CE2	2.47	0.49
1:A:184:GLY:HA2	1:A:186:TRP:NE1	2.28	0.49
1:A:118:SER:OG	1:A:120:SER:O	2.30	0.48
1:A:164:VAL:HG21	1:C:21:TYR:OH	2.14	0.48
1:B:140:TRP:CZ2	1:B:214:GLU:CG	2.96	0.48
1:B:85:VAL:HG11	1:B:108:GLN:HB2	1.96	0.47
1:B:21:TYR:O	1:B:71:ASN:HB3	2.16	0.46
1:B:112:PHE:O	1:B:114:ALA:N	2.49	0.46
1:B:13:GLU:HA	1:B:80:ALA:HB3	1.98	0.45
1:B:13:GLU:OE1	1:B:13:GLU:N	2.48	0.45
1:C:30:VAL:HG11	1:C:73:MET:HG3	1.99	0.45
1:A:143:GLN:N	1:A:207:GLN:O	2.49	0.43
1:A:5:TRP:HB3	1:A:102:LYS:HG3	1.99	0.43
1:B:140:TRP:HZ2	1:B:214:GLU:OE2	2.02	0.43
1:B:64:LEU:HG	1:B:76:PHE:CE1	2.53	0.42
1:B:173:PHE:CE2	1:B:175:ARG:HB2	2.54	0.42
1:B:140:TRP:CD2	1:B:140:TRP:N	2.87	0.42
1:A:22:PRO:O	1:A:24:MET:HG2	2.19	0.42
1:C:85:VAL:HG21	1:C:108:GLN:HB2	2.03	0.41
1:A:30:VAL:HB	1:A:45:PHE:HB3	2.03	0.41
1:B:22:PRO:HG2	1:B:24:MET:SD	2.62	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	219/232 (94%)	207 (94%)	10 (5%)	2 (1%)	14	27
1	B	214/232 (92%)	199 (93%)	14 (6%)	1 (0%)	24	43
1	C	101/232 (44%)	95 (94%)	6 (6%)	0	100	100
All	All	534/696 (77%)	501 (94%)	30 (6%)	3 (1%)	21	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	B	113	GLU
1	A	173	PHE

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	200/210 (95%)	199 (100%)	1 (0%)	81	92
1	B	198/210 (94%)	197 (100%)	1 (0%)	81	92
1	C	95/210 (45%)	95 (100%)	0	100	100
All	All	493/630 (78%)	491 (100%)	2 (0%)	84	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	ARG
1	B	140	TRP

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	49	HIS
1	B	154	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 oligosaccharides 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	221/232 (95%)	1.21	47 (21%) 2 2	30, 57, 129, 157	0
1	B	218/232 (93%)	2.02	92 (42%) 0 0	31, 73, 121, 149	0
1	C	105/232 (45%)	2.24	49 (46%) 0 0	61, 85, 139, 185	0
All	All	544/696 (78%)	1.74	188 (34%) 1 1	30, 71, 129, 185	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	VAL	9.3
1	B	114	ALA	9.2
1	C	4	LEU	7.4
1	C	21	TYR	6.7
1	C	69	ALA	6.3
1	C	67	THR	6.2
1	B	4	LEU	6.1
1	C	68	MET	6.0
1	B	115	ALA	6.0
1	C	66	SER	6.0
1	C	3	VAL	5.9
1	A	223	ALA	5.7
1	A	163	LEU	5.7
1	B	66	SER	5.6
1	B	113	GLU	5.6
1	B	181	CYS	5.4
1	B	164	VAL	5.3
1	B	112	PHE	5.1
1	C	71	ASN	4.9
1	A	141	PRO	4.8
1	B	69	ALA	4.8
1	A	139	THR	4.8
1	A	186	TRP	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	116	VAL	4.8
1	B	210	ALA	4.7
1	C	78	ARG	4.6
1	B	110	ASP	4.6
1	B	64	LEU	4.6
1	B	140	TRP	4.5
1	B	111	SER	4.5
1	B	67	THR	4.4
1	C	64	LEU	4.3
1	C	109	SER	4.3
1	A	140	TRP	4.3
1	B	169	PHE	4.3
1	C	92	LEU	4.3
1	B	223	ALA	4.2
1	A	210	ALA	4.1
1	B	107	VAL	4.1
1	B	35	ILE	4.1
1	B	88	TYR	4.1
1	A	162	ASN	4.0
1	A	183	HIS	4.0
1	B	65	ASN	4.0
1	C	65	ASN	4.0
1	B	87	TYR	4.0
1	A	211	GLY	4.0
1	A	182	SER	4.0
1	A	38	GLN	3.9
1	B	60	ARG	3.8
1	C	70	SER	3.8
1	B	9	VAL	3.8
1	B	71	ASN	3.8
1	B	11	PHE	3.7
1	A	167	ARG	3.7
1	C	5	TRP	3.7
1	B	185	ARG	3.7
1	A	164	VAL	3.7
1	A	138	MET	3.7
1	B	106	VAL	3.6
1	A	209	SER	3.6
1	A	112	PHE	3.6
1	A	169	PHE	3.6
1	B	78	ARG	3.5
1	B	10	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	106	VAL	3.5
1	B	68	MET	3.5
1	B	21	TYR	3.5
1	A	213	ASN	3.5
1	B	14	ASN	3.5
1	B	70	SER	3.5
1	C	27	LEU	3.4
1	A	185	ARG	3.4
1	B	40	ASP	3.4
1	A	160	TYR	3.4
1	A	168	ASN	3.4
1	C	107	VAL	3.4
1	B	109	SER	3.4
1	B	72	ASN	3.3
1	A	142	VAL	3.3
1	B	176	GLN	3.2
1	A	205	TYR	3.2
1	B	211	GLY	3.2
1	B	182	SER	3.2
1	B	85	VAL	3.2
1	C	73	MET	3.2
1	A	145	VAL	3.2
1	C	9	VAL	3.2
1	B	86	GLY	3.1
1	B	196	VAL	3.1
1	C	98	GLY	3.1
1	B	62	TYR	3.1
1	C	72	ASN	3.1
1	B	108	GLN	3.0
1	B	17	LEU	3.0
1	C	39	GLN	3.0
1	C	108	GLN	3.0
1	B	161	CYS	3.0
1	B	163	LEU	3.0
1	C	11	PHE	2.9
1	A	212	GLU	2.9
1	A	170	THR	2.8
1	B	80	ALA	2.8
1	B	83	ASP	2.8
1	B	138	MET	2.8
1	C	87	TYR	2.8
1	B	168	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	76	PHE	2.7
1	C	37	THR	2.7
1	C	36	GLY	2.7
1	B	174	PRO	2.7
1	C	79	ASN	2.7
1	B	125	GLU	2.7
1	A	110	ASP	2.7
1	C	62	TYR	2.7
1	C	12	ALA	2.7
1	C	110	ASP	2.6
1	A	161	CYS	2.6
1	A	165	HIS	2.6
1	A	24	MET	2.6
1	B	61	VAL	2.6
1	C	8	SER	2.6
1	B	36	GLY	2.6
1	B	203	ARG	2.6
1	C	25	GLY	2.6
1	C	93	TYR	2.6
1	A	184	GLY	2.5
1	C	99	THR	2.5
1	B	162	ASN	2.5
1	B	16	SER	2.5
1	B	212	GLU	2.5
1	A	177	ILE	2.5
1	B	33	PHE	2.5
1	C	100	TRP	2.4
1	B	201	LEU	2.4
1	B	13	GLU	2.4
1	C	81	SER	2.4
1	B	24	MET	2.4
1	B	159	THR	2.4
1	A	193	ASP	2.4
1	B	151	GLN	2.4
1	A	116	VAL	2.4
1	B	55	LYS	2.4
1	B	82	GLU	2.4
1	B	81	SER	2.3
1	C	60	ARG	2.3
1	B	84	ASP	2.3
1	A	173	PHE	2.3
1	C	103	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	79	ASN	2.3
1	B	141	PRO	2.3
1	A	218	MET	2.3
1	B	77	PHE	2.3
1	A	216	PHE	2.3
1	B	79	ASN	2.2
1	B	15	MET	2.2
1	C	104	ILE	2.2
1	B	186	TRP	2.2
1	B	222	VAL	2.2
1	C	96	PRO	2.2
1	B	34	LYS	2.2
1	B	195	THR	2.2
1	B	153	ARG	2.2
1	B	130	VAL	2.2
1	A	180	ASN	2.2
1	C	80	ALA	2.2
1	C	38	GLN	2.2
1	B	139	THR	2.2
1	B	202	TYR	2.2
1	C	35	ILE	2.2
1	B	39	GLN	2.1
1	B	105	GLN	2.1
1	C	59	GLU	2.1
1	B	8	SER	2.1
1	C	6	HIS	2.1
1	A	158	LEU	2.1
1	A	192	PRO	2.1
1	B	126	PRO	2.1
1	B	20	VAL	2.1
1	A	64	LEU	2.1
1	A	166	GLY	2.1
1	A	207	GLN	2.1
1	B	37	THR	2.1
1	A	40	ASP	2.1
1	A	146	ARG	2.0
1	C	82	GLU	2.0
1	B	180	ASN	2.0
1	C	57	TYR	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 oligosaccharides 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.