



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:58 AM UTC

PDB ID : 5Z78 / pdb_00005z78
Title : Structure of TIRR/53BP1 complex
Authors : Dai, Y.X.; Shan, S.
Deposited on : 2018-01-27
Resolution : 1.76 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

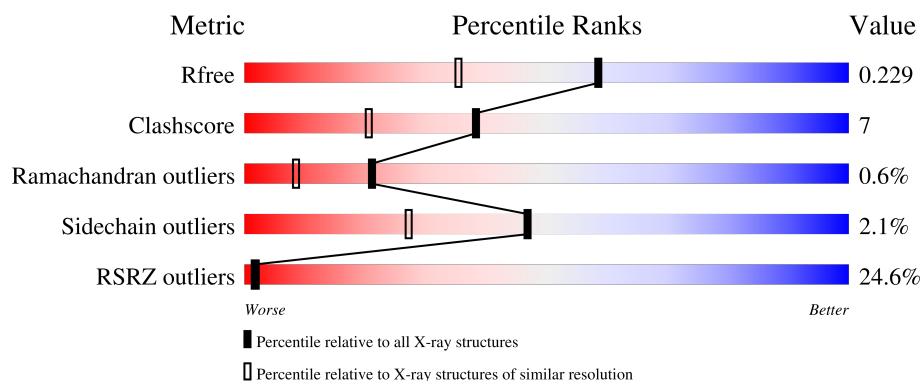
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	209	12% 89% 6% 5%
1	B	209	13% 85% 9% 6%
2	C	123	59% 64% 28% • • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4192 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 Tudor-interacting repair regulator protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	197	Total	C	N	O	S	0	0	0
			1545	989	278	270	8			
1	A	199	Total	C	N	O	S	0	0	0
			1561	998	280	274	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	GLY	-	expression tag	UNP Q8VHN8
B	4	HIS	-	expression tag	UNP Q8VHN8
B	5	MET	-	expression tag	UNP Q8VHN8
A	3	GLY	-	expression tag	UNP Q8VHN8
A	4	HIS	-	expression tag	UNP Q8VHN8
A	5	MET	-	expression tag	UNP Q8VHN8

- Molecule 2 is a protein called TP53-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	121	Total	C	N	O	S	0	0	0
			968	618	164	182	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1481	GLY	-	expression tag	UNP Q12888
C	1482	HIS	-	expression tag	UNP Q12888
C	1483	MET	-	expression tag	UNP Q12888

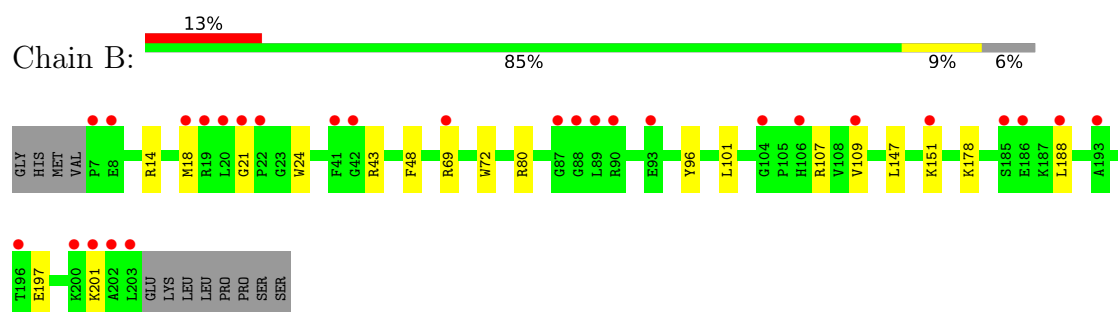
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	56	Total 56	O 56	0	0
3	A	53	Total 53	O 53	0	0
3	C	9	Total 9	O 9	0	0

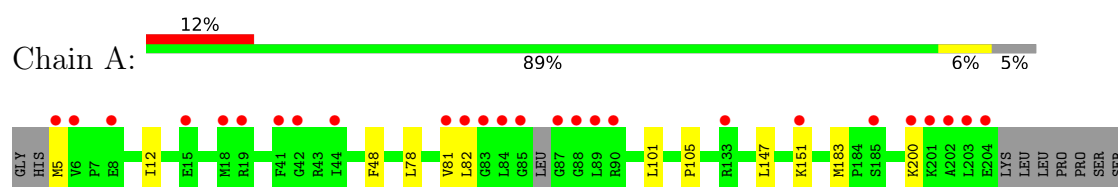
3 Residue-property plots [i](#)

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.

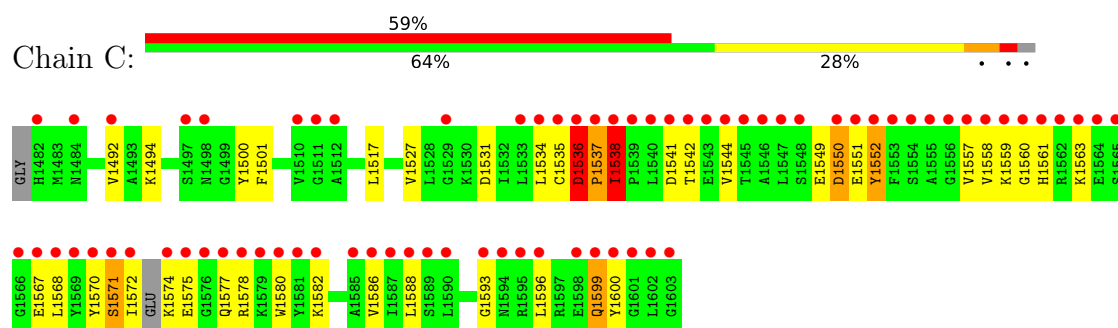
- Molecule 1: Tudor-interacting repair regulator protein



- Molecule 1: Tudor-interacting repair regulator protein



- Molecule 2: TP53-binding protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	167.11Å 167.11Å 46.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.63 – 1.76 40.63 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.63-1.76) 99.9 (40.63-1.76)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.206 , 0.222 0.223 , 0.229	Depositor DCC
R_{free} test set	3717 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4192	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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	0.45	0/1595	0.73	0/2150
1	B	0.48	0/1580	0.78	2/2131 (0.1%)
2	C	0.70	2/987 (0.2%)	1.07	3/1324 (0.2%)
All	All	0.53	2/4162 (0.0%)	0.84	5/5605 (0.1%)

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
2	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1536	ASP	C-N	6.24	1.41	1.33
2	C	1538	ILE	C-N	5.61	1.40	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1538	ILE	CA-C-N	-7.99	112.54	120.21
2	C	1538	ILE	C-N-CA	-7.99	112.54	120.21
1	B	21	GLY	CA-C-N	6.90	126.53	119.56
1	B	21	GLY	C-N-CA	6.90	126.53	119.56
2	C	1537	PRO	CA-N-CD	-5.14	104.81	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1536	ASP	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	1561	0	1577	7	0
1	B	1545	0	1566	10	0
2	C	968	0	952	40	0
3	A	53	0	0	0	0
3	B	56	0	0	0	0
3	C	9	0	0	0	0
All	All	4192	0	4095	56	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 7.

All (56) 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:1535:CYS:SG	2:C:1600:TYR:CG	2.37	1.16
2:C:1535:CYS:SG	2:C:1600:TYR:CB	2.43	1.06
2:C:1535:CYS:SG	2:C:1600:TYR:HB3	1.97	1.04
2:C:1550:ASP:O	2:C:1552:TYR:N	1.91	1.02
2:C:1559:LYS:HE3	2:C:1578:ARG:HG3	1.52	0.90
2:C:1571:SER:OG	2:C:1571:SER:O	1.88	0.87
2:C:1492:VAL:HG12	2:C:1501:PHE:HB3	1.73	0.71
2:C:1559:LYS:N	2:C:1571:SER:OG	2.23	0.70
2:C:1538:ILE:HG12	2:C:1570:TYR:OH	1.91	0.70
1:B:43:ARG:NH1	1:B:151:LYS:HE3	2.12	0.65
2:C:1557:VAL:H	2:C:1578:ARG:HH22	1.44	0.64
2:C:1527:VAL:HG13	2:C:1531:ASP:HB2	1.81	0.63
2:C:1535:CYS:SG	2:C:1600:TYR:CD2	2.94	0.61
2:C:1501:PHE:HB2	2:C:1588:LEU:HB2	1.83	0.61
2:C:1536:ASP:HB2	2:C:1537:PRO:CD	2.32	0.60
2:C:1549:GLU:HA	2:C:1549:GLU:OE1	2.01	0.59
2:C:1571:SER:HB2	2:C:1580:TRP:HZ3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LEU:HD23	1:B:109:VAL:HG12	1.86	0.57
2:C:1550:ASP:C	2:C:1552:TYR:H	2.05	0.56
2:C:1494:LYS:NZ	2:C:1531:ASP:OD1	2.38	0.55
2:C:1572:ILE:C	2:C:1578:ARG:NH1	2.66	0.54
2:C:1536:ASP:CB	2:C:1537:PRO:CD	2.85	0.54
1:B:18:MET:SD	1:B:69:ARG:NH1	2.81	0.54
2:C:1559:LYS:CE	2:C:1578:ARG:HG3	2.32	0.53
1:B:197:GLU:OE2	1:B:201:LYS:HE3	2.09	0.53
2:C:1561:HIS:HB3	2:C:1568:LEU:HD11	1.90	0.53
2:C:1527:VAL:CG1	2:C:1531:ASP:HB2	2.39	0.52
2:C:1560:GLY:O	2:C:1571:SER:HB3	2.10	0.52
1:B:24:TRP:CD2	1:B:107:ARG:HB3	2.45	0.51
1:B:178:LYS:HG3	1:B:188:LEU:CD1	2.40	0.51
2:C:1542:THR:HG23	2:C:1596:LEU:HD11	1.93	0.51
2:C:1536:ASP:CB	2:C:1537:PRO:HD3	2.41	0.50
2:C:1538:ILE:HG13	2:C:1570:TYR:CZ	2.47	0.50
2:C:1538:ILE:CG1	2:C:1570:TYR:CZ	2.95	0.49
2:C:1570:TYR:HB2	2:C:1586:VAL:HG21	1.96	0.48
1:B:72:TRP:CH2	1:B:80:ARG:HD3	2.49	0.47
1:B:178:LYS:HG3	1:B:188:LEU:HD12	1.96	0.47
1:A:151:LYS:HE3	1:A:151:LYS:HB3	1.61	0.46
1:B:14:ARG:HG3	1:B:96:TYR:CZ	2.51	0.46
1:A:105:PRO:HB3	2:C:1500:TYR:CE2	2.51	0.46
2:C:1567:GLU:OE1	2:C:1582:LYS:NZ	2.43	0.46
2:C:1588:LEU:HD13	2:C:1593:GLY:HA2	1.97	0.45
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.66	0.45
2:C:1574:LYS:O	2:C:1577:GLN:N	2.49	0.44
2:C:1538:ILE:HG12	2:C:1538:ILE:H	1.53	0.44
2:C:1599:GLN:HB3	2:C:1600:TYR:CD2	2.52	0.44
1:A:48:PHE:HB2	1:A:147:LEU:HD12	1.99	0.43
1:B:48:PHE:HB2	1:B:147:LEU:HD12	2.00	0.43
1:A:78:LEU:HA	1:A:81:VAL:HG22	1.99	0.43
2:C:1534:LEU:N	2:C:1600:TYR:O	2.47	0.43
1:A:183:MET:HB3	1:A:183:MET:HE3	1.85	0.42
2:C:1538:ILE:HG12	2:C:1570:TYR:CZ	2.56	0.41
1:A:12:ILE:HD13	1:A:101:LEU:HD21	2.02	0.41
2:C:1541:ASP:N	2:C:1558:VAL:O	2.46	0.41
2:C:1536:ASP:HB2	2:C:1537:PRO:HD3	2.00	0.41
2:C:1544:VAL:HG21	2:C:1586:VAL:HG13	2.03	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	195/209 (93%)	189 (97%)	6 (3%)	0	100	100
1	B	195/209 (93%)	190 (97%)	5 (3%)	0	100	100
2	C	117/123 (95%)	108 (92%)	6 (5%)	3 (3%)	4	0
All	All	507/541 (94%)	487 (96%)	17 (3%)	3 (1%)	21	8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1551	GLU
2	C	1575	GLU
2	C	1536	ASP

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	164/173 (95%)	162 (99%)	2 (1%)	63	49
1	B	162/173 (94%)	162 (100%)	0	100	100
2	C	102/103 (99%)	95 (93%)	7 (7%)	14	2
All	All	428/449 (95%)	419 (98%)	9 (2%)	47	27

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	200	LYS
2	C	1517	LEU
2	C	1538	ILE
2	C	1550	ASP
2	C	1552	TYR
2	C	1563	LYS
2	C	1571	SER
2	C	1599	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	199/209 (95%)	0.71	26 (13%) 7 8	22, 33, 53, 66	0
1	B	197/209 (94%)	0.80	28 (14%) 6 7	23, 32, 51, 65	0
2	C	121/123 (98%)	2.67	73 (60%) 0 0	24, 49, 83, 101	0
All	All	517/541 (95%)	1.20	127 (24%) 2 2	22, 35, 72, 101	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1536	ASP	8.7
2	C	1580	TRP	8.2
2	C	1552	TYR	7.9
2	C	1550	ASP	7.8
1	B	7	PRO	7.0
2	C	1535	CYS	6.8
2	C	1572	ILE	6.7
2	C	1551	GLU	6.7
1	B	203	LEU	5.4
1	A	82	LEU	5.4
2	C	1581	TYR	5.3
2	C	1576	GLY	5.2
2	C	1540	LEU	5.1
2	C	1569	TYR	5.1
2	C	1482	HIS	5.0
2	C	1579	LYS	4.8
2	C	1565	SER	4.8
2	C	1510	VAL	4.8
2	C	1574	LYS	4.6
1	A	41	PHE	4.5
2	C	1577	GLN	4.5
2	C	1590	LEU	4.5
2	C	1603	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
2	C	1570	TYR	4.5
2	C	1600	TYR	4.5
2	C	1538	ILE	4.4
1	B	88	GLY	4.4
2	C	1567	GLU	4.4
2	C	1558	VAL	4.3
1	A	5	MET	4.3
2	C	1541	ASP	4.3
1	A	85	GLY	4.3
2	C	1568	LEU	4.3
1	B	87	GLY	4.2
2	C	1596	LEU	4.1
1	B	41	PHE	4.1
1	A	84	LEU	4.0
2	C	1566	GLY	3.8
2	C	1542	THR	3.8
1	A	204	GLU	3.8
2	C	1557	VAL	3.7
1	B	186	GLU	3.7
1	A	202	ALA	3.6
1	A	83	GLY	3.6
1	B	201	LYS	3.6
2	C	1559	LYS	3.6
1	B	19	ARG	3.5
1	A	203	LEU	3.5
2	C	1582	LYS	3.5
2	C	1537	PRO	3.5
2	C	1601	GLY	3.5
1	A	81	VAL	3.5
2	C	1571	SER	3.5
2	C	1556	GLY	3.4
1	B	200	LYS	3.4
2	C	1543	GLU	3.4
2	C	1554	SER	3.4
1	A	88	GLY	3.3
1	B	202	ALA	3.3
1	B	104	GLY	3.3
2	C	1575	GLU	3.3
2	C	1555	ALA	3.3
1	B	18	MET	3.2
1	B	8	GLU	3.2
2	C	1599	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	87	GLY	3.2
2	C	1512	ALA	3.1
2	C	1594	ASN	3.1
1	B	20	LEU	3.1
2	C	1497	SER	3.0
2	C	1578	ARG	3.0
2	C	1598	GLU	2.9
1	B	42	GLY	2.9
2	C	1539	PRO	2.9
2	C	1593	GLY	2.9
1	A	200	LYS	2.8
1	B	89	LEU	2.8
2	C	1548	SER	2.8
2	C	1602	LEU	2.8
2	C	1560	GLY	2.8
2	C	1562	ARG	2.8
1	A	89	LEU	2.8
2	C	1561	HIS	2.7
2	C	1553	PHE	2.7
2	C	1544	VAL	2.7
2	C	1588	LEU	2.6
1	A	44	ILE	2.6
1	A	15	GLU	2.6
2	C	1585	ALA	2.6
1	B	188	LEU	2.6
1	B	22	PRO	2.6
2	C	1564	GLU	2.6
1	B	106	HIS	2.6
1	B	109	VAL	2.6
1	B	90	ARG	2.5
1	B	93	GLU	2.5
1	B	185	SER	2.5
2	C	1533	LEU	2.5
2	C	1546	ALA	2.5
1	A	201	LYS	2.5
2	C	1511	GLY	2.5
1	B	69	ARG	2.5
1	A	151	LYS	2.4
2	C	1534	LEU	2.4
1	B	151	LYS	2.4
1	A	90	ARG	2.4
2	C	1498	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	1595	ARG	2.3
2	C	1545	THR	2.3
1	B	21	GLY	2.3
1	A	18	MET	2.2
1	B	196	THR	2.2
1	A	133	ARG	2.2
2	C	1492	VAL	2.2
2	C	1586	VAL	2.2
1	A	8	GLU	2.2
1	A	42	GLY	2.2
1	A	6	VAL	2.1
2	C	1589	SER	2.1
2	C	1587	ILE	2.1
1	B	193	ALA	2.1
2	C	1529	GLY	2.1
2	C	1484	ASN	2.1
1	A	185	SER	2.1
1	A	19	ARG	2.1
2	C	1547	LEU	2.0
2	C	1563	LYS	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.