



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 01:54 AM UTC

PDB ID : 5XHF / pdb_00005xhf
Title : Crystal structure of Trastuzumab Fab fragment bearing p-azido-L-phenylalanine
Authors : Kuratani, M.; Yanagisawa, T.; Sakamoto, K.; Yokoyama, S.
Deposited on : 2017-04-20
Resolution : 3.21 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

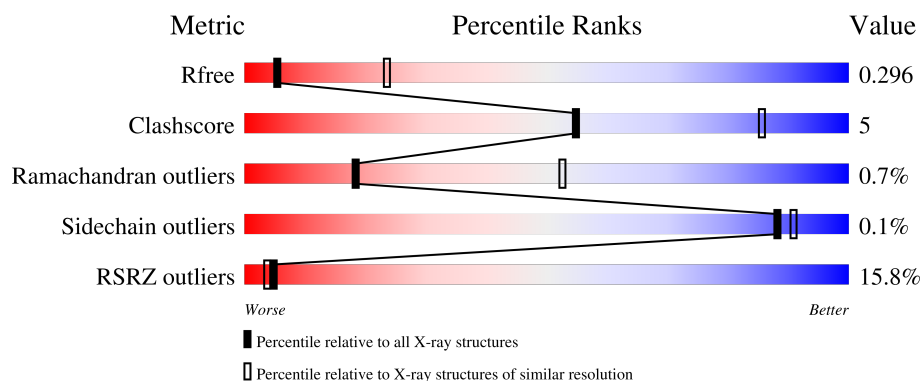
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	214	
1	C	214	
2	B	220	
2	D	220	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6565 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 polypeptide (L chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1648	1033	278	332	5			
1	C	214	Total	C	N	O	S	0	0	0
			1654	1036	279	333	6			

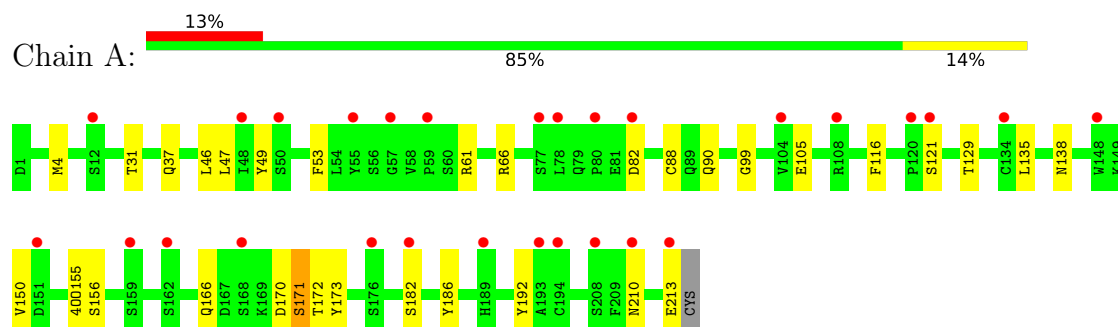
- Molecule 2 is a protein called polypeptide (H chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1611	1021	271	313	6			
2	D	220	Total	C	N	O	S	0	1	0
			1652	1044	278	323	7			

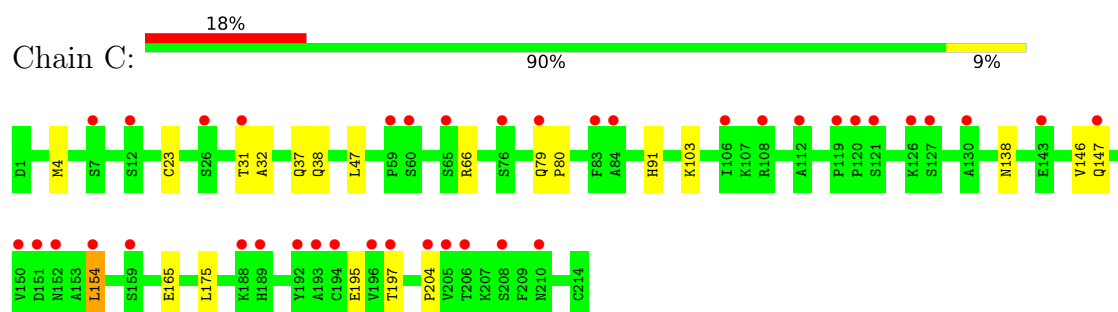
3 Residue-property plots

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.

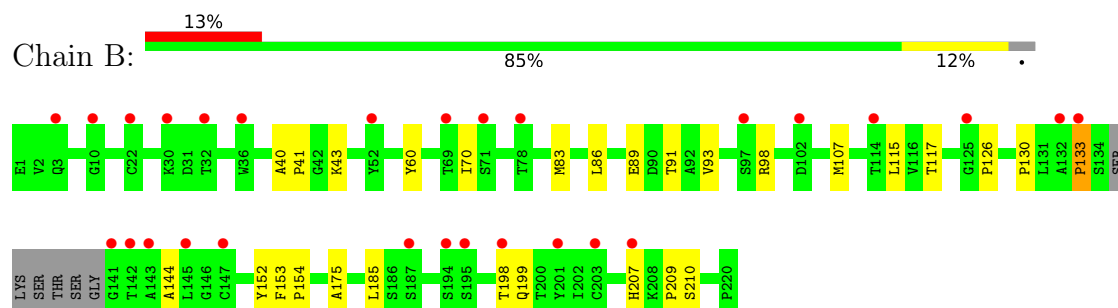
- Molecule 1: polypeptide (L chain)



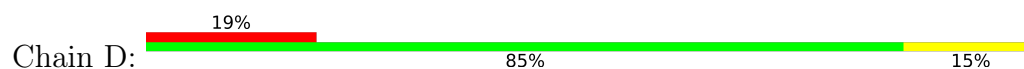
- Molecule 1: polypeptide (L chain)

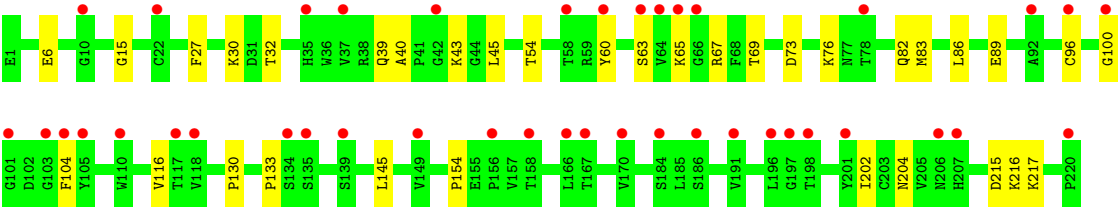


- Molecule 2: polypeptide (H chain)



- Molecule 2: polypeptide (H chain)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.84Å 80.07Å 85.79Å 113.67° 92.35° 102.78°	Depositor
Resolution (Å)	42.44 – 3.21 42.44 – 3.21	Depositor EDS
% Data completeness (in resolution range)	98.4 (42.44-3.21) 98.4 (42.44-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.219 , 0.297 0.222 , 0.296	Depositor DCC
R_{free} test set	1476 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6565	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.17% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4OO

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	0.09	0/1670	0.26	0/2269
1	C	0.09	0/1676	0.27	0/2277
2	B	0.08	0/1652	0.26	0/2253
2	D	0.09	0/1697	0.25	0/2314
All	All	0.09	0/6695	0.26	0/9113

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	1648	0	1595	17	0
1	C	1654	0	1600	11	0
2	B	1611	0	1567	16	0
2	D	1652	0	1610	20	0
All	All	6565	0	6372	62	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 5.

All (62) 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:D:83:MET:HB3	2:D:86:LEU:HD21	1.71	0.70
2:D:100:GLY:HA3	2:D:104:PHE:HB3	1.73	0.68
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.78	0.66
1:A:170:ASP:O	1:A:172:THR:N	2.32	0.63
1:A:4:MET:HE3	1:A:90:GLN:HB3	1.82	0.62
2:D:202:ILE:HG12	2:D:217:LYS:HA	1.83	0.61
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.82	0.61
2:D:69:THR:HB	2:D:82:GLN:HB3	1.84	0.59
2:D:60:TYR:O	2:D:65:LYS:NZ	2.36	0.57
2:D:30:LYS:O	2:D:54:THR:OG1	2.23	0.57
2:B:91:THR:HG23	2:B:117:THR:HA	1.88	0.56
2:B:207:HIS:ND1	2:B:210:SER:OG	2.40	0.54
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.90	0.53
1:C:147:GLN:HG3	1:C:154:LEU:HD11	1.90	0.53
1:C:197:THR:HG22	1:C:204:PRO:HB3	1.90	0.53
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.90	0.53
1:A:121:SER:OG	2:B:130:PRO:O	2.27	0.51
2:D:133:PRO:HG3	2:D:145:LEU:HB3	1.92	0.51
2:B:89:GLU:OE1	2:B:89:GLU:N	2.40	0.51
2:D:40:ALA:HB3	2:D:43:LYS:HB2	1.92	0.51
1:C:146:VAL:HG21	1:C:175:LEU:HD22	1.91	0.51
2:B:93:VAL:HA	2:B:115:LEU:HA	1.93	0.51
2:D:63:SER:O	2:D:67:ARG:NH2	2.44	0.51
1:A:116:PHE:HB2	1:A:135:LEU:HB3	1.93	0.50
2:D:89:GLU:OE1	2:D:89:GLU:N	2.45	0.50
1:A:105:GLU:OE1	1:A:173:TYR:OH	2.25	0.49
1:A:150:VAL:HG21	1:A:155:4OO:H12	1.95	0.48
1:A:31:THR:HG22	1:A:66:ARG:HD2	1.94	0.48
2:D:69:THR:O	2:D:82:GLN:N	2.46	0.47
1:C:103:LYS:NZ	1:C:165:GLU:OE1	2.41	0.47
2:D:15:GLY:N	2:D:86:LEU:O	2.45	0.47
1:A:155:4OO:H9	1:A:156:SER:H	1.80	0.46
2:D:27:PHE:HE2	2:D:32:THR:HG21	1.79	0.46
1:A:210:ASN:HB2	1:A:213:GLU:HB2	1.97	0.46
2:B:126:PRO:HB3	2:B:152:TYR:HB3	1.97	0.46
2:D:83:MET:HE1	2:D:116:VAL:HG11	1.96	0.45
2:B:153:PHE:HA	2:B:154:PRO:HA	1.74	0.45
1:C:31:THR:HG22	1:C:66:ARG:HD2	1.99	0.44
1:A:61:ARG:NH1	1:A:82:ASP:OD1	2.48	0.44
2:B:93:VAL:HG22	2:B:115:LEU:HB3	1.99	0.44
1:C:147:GLN:HB3	1:C:195:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:TYR:O	1:A:53:PHE:HB2	2.18	0.44
2:B:207:HIS:CD2	2:B:209:PRO:HD2	2.53	0.43
2:B:98:ARG:O	2:B:107:MET:HA	2.19	0.43
2:B:175:ALA:HB2	2:B:185:LEU:HD23	2.00	0.42
2:B:60:TYR:CZ	2:B:70:ILE:HG22	2.54	0.42
2:D:6:GLU:HG2	2:D:96[B]:CYS:SG	2.59	0.42
2:D:39:GLN:HB2	2:D:45:LEU:HD23	2.01	0.42
2:D:130:PRO:HD3	2:D:216:LYS:HE2	2.01	0.42
2:D:204:ASN:ND2	2:D:215:ASP:OD1	2.35	0.42
2:B:133:PRO:HB3	2:B:144:ALA:O	2.20	0.42
2:D:73:ASP:HB3	2:D:76:LYS:HB2	2.02	0.42
1:A:88:CYS:O	1:A:99:GLY:N	2.53	0.41
1:A:46:LEU:HD21	1:A:49:TYR:HB3	2.02	0.41
1:C:32:ALA:HB1	1:C:91:HIS:CE1	2.55	0.41
1:C:38:GLN:OE1	2:D:39:GLN:NE2	2.51	0.41
1:A:186:TYR:O	1:A:192:TYR:OH	2.34	0.41
1:A:129:THR:HA	1:A:182:SER:HA	2.02	0.41
1:A:166:GLN:NE2	1:A:171:SER:HB3	2.36	0.41
2:B:198:THR:OG1	2:B:199:GLN:N	2.54	0.40
1:C:79:GLN:HB3	1:C:80:PRO:HD2	2.03	0.40
1:C:4:MET:HG3	1:C:23:CYS:SG	2.61	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	210/214 (98%)	194 (92%)	14 (7%)	2 (1%)	12	45
1	C	211/214 (99%)	196 (93%)	14 (7%)	1 (0%)	24	59
2	B	210/220 (96%)	196 (93%)	12 (6%)	2 (1%)	12	45
2	D	219/220 (100%)	207 (94%)	11 (5%)	1 (0%)	24	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	850/868 (98%)	793 (93%)	51 (6%)	6 (1%)	18	52

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	SER
1	C	138	ASN
1	A	138	ASN
2	B	133	PRO
2	B	41	PRO
2	D	154	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	187/188 (100%)	187 (100%)	0	100	100
1	C	188/188 (100%)	187 (100%)	1 (0%)	81	85
2	B	176/181 (97%)	176 (100%)	0	100	100
2	D	182/181 (101%)	182 (100%)	0	100	100
All	All	733/738 (99%)	732 (100%)	1 (0%)	88	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	154	LEU

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

Mol	Chain	Res	Type
1	A	89	GLN
2	B	171	HIS
1	C	138	ASN

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Mol	Chain	Res	Type
2	D	112	GLN
2	D	178	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	212/214 (99%)	1.26	28 (13%)	7 6	16, 37, 57, 77	0
1	C	213/214 (99%)	1.32	39 (18%)	3 3	17, 38, 64, 87	0
2	B	214/220 (97%)	1.15	28 (13%)	7 6	13, 28, 59, 76	0
2	D	220/220 (100%)	1.28	41 (18%)	3 3	13, 30, 68, 93	1 (0%)
All	All	859/868 (98%)	1.25	136 (15%)	5 4	13, 33, 62, 93	1 (0%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	101	GLY	4.3
1	A	59	PRO	4.1
2	B	22	CYS	3.8
1	C	83	PHE	3.6
1	C	204	PRO	3.6
1	A	12	SER	3.6
1	C	12	SER	3.5
1	A	210	ASN	3.4
1	C	26	SER	3.4
2	B	195	SER	3.3
2	D	170	VAL	3.3
1	A	208	SER	3.2
1	C	112	ALA	3.2
1	C	59	PRO	3.1
1	C	106	ILE	3.1
1	C	206	THR	3.0
1	A	78	LEU	3.0
1	C	159	SER	3.0
1	A	134	CYS	3.0
2	D	65	LYS	2.9
2	D	103	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	92	ALA	2.8
1	C	121	SER	2.8
2	B	97	SER	2.8
1	A	80	PRO	2.8
1	A	151	ASP	2.8
1	C	76	SER	2.8
2	D	207	HIS	2.7
2	D	22	CYS	2.7
2	D	156	PRO	2.7
1	C	208	SER	2.7
2	D	100	GLY	2.7
2	D	201	TYR	2.7
2	D	35	HIS	2.7
2	B	147	CYS	2.7
2	D	186	SER	2.6
1	C	119	PRO	2.6
2	D	42	GLY	2.6
2	B	32	THR	2.6
2	B	69	THR	2.6
2	B	142	THR	2.6
2	D	167	THR	2.6
2	B	201	TYR	2.6
1	C	79	GLN	2.6
1	C	150	VAL	2.6
1	A	194	CYS	2.6
2	B	52	TYR	2.6
2	D	139	SER	2.6
2	D	166	LEU	2.5
1	A	189	HIS	2.5
2	D	158	THR	2.5
1	C	189	HIS	2.5
1	C	147	GLN	2.5
2	B	187	SER	2.5
2	D	134	SER	2.5
2	B	143	ALA	2.5
2	B	3	GLN	2.5
1	A	176	SER	2.4
1	C	65	SER	2.4
1	C	197	THR	2.4
2	D	149	VAL	2.4
1	A	77	SER	2.4
1	C	126	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	198	THR	2.4
2	D	66	GLY	2.4
1	A	193	ALA	2.4
1	C	194	CYS	2.4
1	C	31	THR	2.4
2	B	30	LYS	2.4
1	C	60	SER	2.4
1	A	120	PRO	2.4
2	B	78	THR	2.3
1	C	192	TYR	2.3
2	B	141	GLY	2.3
1	C	154	LEU	2.3
2	D	64	VAL	2.3
2	D	118	VAL	2.3
2	D	191	VAL	2.3
1	A	148	TRP	2.3
2	B	203	CYS	2.3
2	D	206	ASN	2.3
2	B	133	PRO	2.3
1	C	84	ALA	2.3
1	C	7	SER	2.3
1	A	213	GLU	2.3
2	D	135	SER	2.3
2	B	102	ASP	2.3
2	D	58	THR	2.2
2	D	60	TYR	2.2
2	D	63	SER	2.2
2	D	197	GLY	2.2
1	A	121	SER	2.2
2	D	96[A]	CYS	2.2
2	B	114	THR	2.2
2	D	117	THR	2.2
2	D	198	THR	2.2
2	B	194	SER	2.2
1	C	151	ASP	2.2
2	D	104	PHE	2.2
1	C	205	VAL	2.1
2	D	105	TYR	2.1
1	A	162	SER	2.1
1	A	168	SER	2.1
1	C	193	ALA	2.1
2	D	184	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	125	GLY	2.1
2	D	10	GLY	2.1
1	C	143	GLU	2.1
1	C	210	ASN	2.1
2	B	36	TRP	2.1
1	A	55	TYR	2.1
1	A	57	GLY	2.1
1	C	120	PRO	2.1
2	D	220	PRO	2.1
1	A	50	SER	2.1
2	D	110	TRP	2.1
1	A	48	ILE	2.1
2	B	145	LEU	2.1
1	A	182	SER	2.1
1	C	127	SER	2.1
1	A	104	VAL	2.1
1	C	152	ASN	2.1
2	B	207	HIS	2.1
2	D	78	THR	2.1
2	B	10	GLY	2.1
1	C	196	VAL	2.0
1	A	159	SER	2.0
2	B	71	SER	2.0
1	A	108	ARG	2.0
1	C	108	ARG	2.0
2	D	196	LEU	2.0
1	A	82	ASP	2.0
1	C	130	ALA	2.0
2	B	132	ALA	2.0
1	C	188	LYS	2.0
2	D	37	VAL	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.