



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:37 AM GMT

PDB ID : 2XRA
Title : crystal structure of the HK20 Fab in complex with a gp41 mimetic 5- Helix
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Deposited on : 2010-09-13
Resolution : 2.30 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

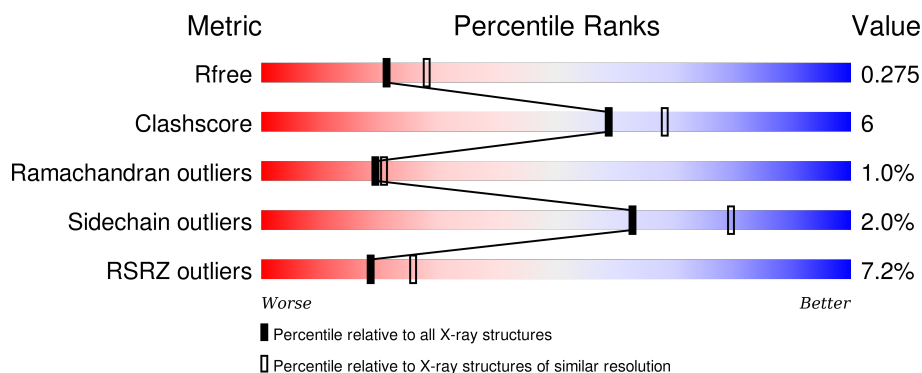
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	228	<div> <div>6%</div> <div>86%</div> <div>11%</div> </div>
2	H	223	<div> <div>5%</div> <div>83%</div> <div>14%</div> </div>
3	L	215	<div> <div>9%</div> <div>80%</div> <div>19%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5080 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 TRANSMEMBRANE PROTEIN GP41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1647	1029	300	316	2			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	MET	-	EXPRESSION TAG	UNP P04578
A	583	GLY	-	INSERTION	UNP P04578
A	584	GLY	-	INSERTION	UNP P04578
A	585	SER	-	INSERTION	UNP P04578
A	586	GLY	-	INSERTION	UNP P04578
A	587	GLY	-	INSERTION	UNP P04578
A	1663	GLY	-	INSERTION	UNP P04578
A	1664	SER	-	INSERTION	UNP P04578
A	1665	SER	-	INSERTION	UNP P04578
A	2541	GLY	-	INSERTION	UNP P04578
A	2542	GLY	-	INSERTION	UNP P04578
A	3620	GLY	-	INSERTION	UNP P04578
A	3621	GLY	-	INSERTION	UNP P04578
A	3622	SER	-	INSERTION	UNP P04578
A	3623	GLY	-	INSERTION	UNP P04578
A	3624	GLY	-	INSERTION	UNP P04578
A	3663	GLY	-	INSERTION	UNP P04578
A	3664	SER	-	INSERTION	UNP P04578
A	3665	SER	-	INSERTION	UNP P04578
A	3666	GLY	-	INSERTION	UNP P04578
A	3667	GLY	-	INSERTION	UNP P04578
A	4583	LEU	-	EXPRESSION TAG	UNP P04578
A	4584	GLU	-	EXPRESSION TAG	UNP P04578
A	4585	GLY	-	EXPRESSION TAG	UNP P04578
A	4586	GLY	-	EXPRESSION TAG	UNP P04578
A	4587	HIS	-	EXPRESSION TAG	UNP P04578
A	4588	HIS	-	EXPRESSION TAG	UNP P04578

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4589	HIS	-	EXPRESSION TAG	UNP P04578
A	4590	HIS	-	EXPRESSION TAG	UNP P04578
A	4591	HIS	-	EXPRESSION TAG	UNP P04578
A	4592	HIS	-	EXPRESSION TAG	UNP P04578
A	4593	GLY	-	EXPRESSION TAG	UNP P04578

- Molecule 2 is a protein called HK20, HUMAN MONOCLONAL ANTIBODY HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	223	Total	C	N	O	S	0	0	0
			1655	1040	273	332	10			

- Molecule 3 is a protein called HK20, HUMAN MONOCLONAL ANTIBODY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1660	1034	284	336	6			

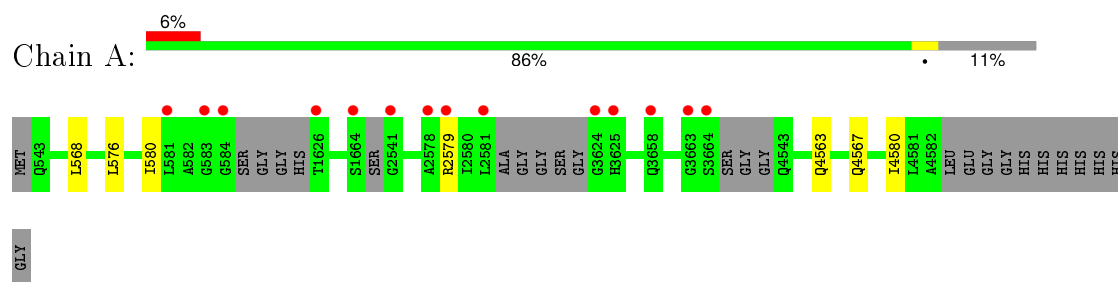
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	H	42	Total	O	0	0
			42	42		
4	L	34	Total	O	0	0
			34	34		

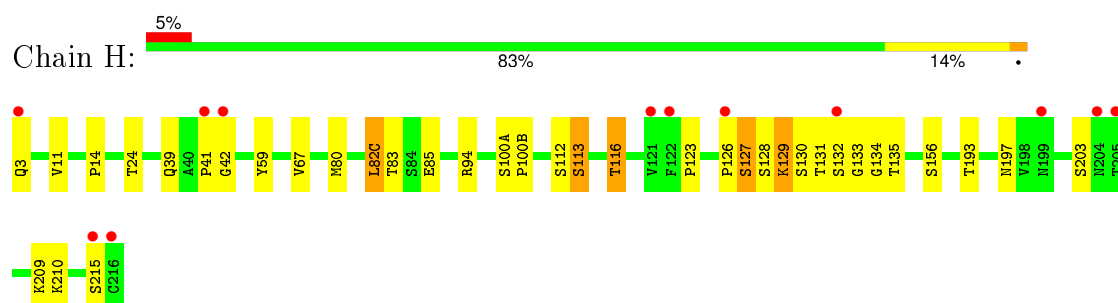
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

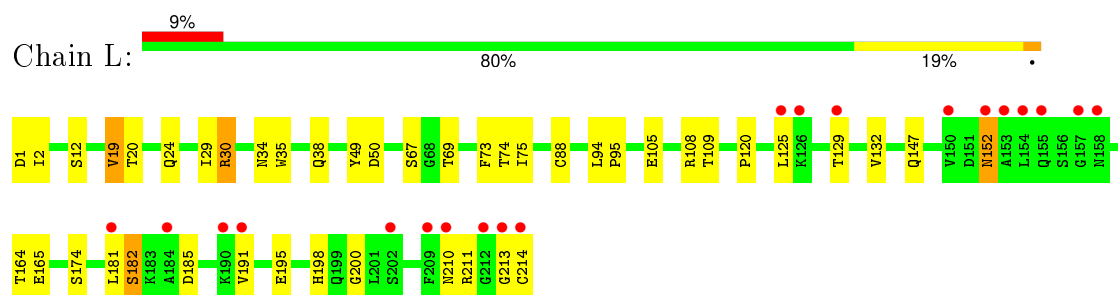
- Molecule 1: TRANSMEMBRANE PROTEIN GP41



- Molecule 2: HK20, HUMAN MONOCLONAL ANTIBODY HEAVY CHAIN



- Molecule 3: HK20, HUMAN MONOCLONAL ANTIBODY LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.95Å 62.71Å 76.61Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	37.63 – 2.30 35.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.2 (37.63-2.30) 93.2 (35.88-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.237 , 0.279 0.232 , 0.275	Depositor DCC
R_{free} test set	1509 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.4	EDS
Estimated twinning fraction	0.020 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29762 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5080	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 7.02% 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	0.51	0/1664	0.58	1/2246 (0.0%)
2	H	0.48	0/1693	0.62	0/2302
3	L	0.45	0/1696	0.55	0/2304
All	All	0.48	0/5053	0.58	1/6852 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	568	LEU	CA-CB-CG	5.36	127.62	115.30

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	1647	0	1647	3	0
2	H	1655	0	1626	29	0
3	L	1660	0	1607	26	0
4	A	42	0	0	0	0
4	H	42	0	0	0	0
4	L	34	0	0	0	0
All	All	5080	0	4880	57	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 6.

All (57) 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:H:126:PRO:HA	2:H:127:SER:HB2	1.40	1.03
2:H:128:SER:HB2	2:H:129:LYS:HB2	1.39	1.01
2:H:126:PRO:HA	2:H:127:SER:CB	1.88	1.01
2:H:156:SER:H	2:H:197:ASN:HD21	1.21	0.84
3:L:164:THR:HG22	3:L:174:SER:H	1.45	0.81
2:H:128:SER:N	2:H:129:LYS:HB3	1.99	0.78
3:L:213:GLY:O	3:L:214:CYS:HB2	1.91	0.71
3:L:213:GLY:O	3:L:214:CYS:CB	2.39	0.70
2:H:112:SER:O	2:H:113:SER:HB3	1.93	0.68
2:H:128:SER:CB	2:H:129:LYS:HB2	2.21	0.67
3:L:19:VAL:HG13	3:L:75:ILE:HB	1.77	0.67
2:H:14:PRO:O	2:H:82(C):LEU:O	2.13	0.67
2:H:131:THR:HA	2:H:135:THR:O	1.97	0.65
2:H:127:SER:HB3	2:H:130:SER:HB3	1.80	0.64
3:L:30:ARG:O	3:L:67:SER:O	2.17	0.62
2:H:126:PRO:HA	2:H:127:SER:HB3	1.77	0.62
3:L:108:ARG:HH11	3:L:109:THR:HG23	1.65	0.61
3:L:147:GLN:HB3	3:L:195:GLU:HB3	1.83	0.60
3:L:181:LEU:O	3:L:182:SER:HB3	2.01	0.59
2:H:126:PRO:CA	2:H:127:SER:CB	2.74	0.58
3:L:94:LEU:N	3:L:95:PRO:HA	2.19	0.58
3:L:198:HIS:CD2	3:L:200:GLY:H	2.22	0.56
3:L:12:SER:HA	3:L:105:GLU:O	2.05	0.56
3:L:34:ASN:ND2	3:L:50:ASP:H	2.05	0.55
2:H:132:SER:H	2:H:133:GLY:HA2	1.71	0.55
2:H:128:SER:N	2:H:129:LYS:CB	2.70	0.54
3:L:181:LEU:O	3:L:182:SER:CB	2.55	0.54
2:H:126:PRO:CA	2:H:127:SER:HB2	2.26	0.53
2:H:3:GLN:O	2:H:24:THR:HA	2.09	0.53
2:H:39:GLN:HE22	3:L:38:GLN:HE22	1.55	0.53
2:H:83:THR:C	2:H:85:GLU:H	2.15	0.51
2:H:123:PRO:HD3	2:H:209:LYS:HE3	1.93	0.50
2:H:128:SER:H	2:H:129:LYS:HB3	1.76	0.50
3:L:129:THR:HA	3:L:182:SER:HA	1.94	0.49
3:L:34:ASN:HD22	3:L:49:TYR:HA	1.77	0.49
3:L:20:THR:HG22	3:L:74:THR:HG23	1.94	0.49
2:H:193:THR:HG23	2:H:210:LYS:HE3	1.94	0.49
2:H:112:SER:O	2:H:113:SER:CB	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:213:GLY:O	3:L:214:CYS:SG	2.72	0.48
3:L:164:THR:HG23	3:L:165:GLU:O	2.15	0.46
1:A:580:ILE:HD13	1:A:2579:ARG:HD2	1.97	0.46
1:A:576:LEU:HD22	1:A:4580:ILE:HD12	1.98	0.45
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.52	0.45
2:H:128:SER:CA	2:H:129:LYS:CB	2.95	0.44
2:H:133:GLY:HA3	2:H:134:GLY:HA2	1.76	0.44
3:L:120:PRO:HD3	3:L:132:VAL:HG22	2.00	0.44
2:H:129:LYS:HG3	2:H:129:LYS:O	2.17	0.43
2:H:100(A):SER:HB3	2:H:100(B):PRO:HD2	1.99	0.43
3:L:24:GLN:HA	3:L:69:THR:O	2.19	0.42
2:H:41:PRO:HA	2:H:42:GLY:HA2	1.58	0.42
1:A:4563:GLN:O	1:A:4567:GLN:HG2	2.20	0.42
3:L:1:ASP:HA	3:L:2:ILE:HA	1.83	0.41
2:H:116:THR:CG2	2:H:203:SER:HB3	2.50	0.41
3:L:29:ILE:O	3:L:30:ARG:C	2.58	0.41
3:L:191:VAL:HG22	3:L:210:ASN:ND2	2.35	0.41
2:H:59:TYR:CD1	2:H:67:VAL:HG13	2.56	0.41
3:L:35:TRP:CE2	3:L:73:PHE:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	193/228 (85%)	191 (99%)	2 (1%)	0	100	100
2	H	221/223 (99%)	207 (94%)	11 (5%)	3 (1%)	14	13
3	L	213/215 (99%)	200 (94%)	10 (5%)	3 (1%)	14	13
All	All	627/666 (94%)	598 (95%)	23 (4%)	6 (1%)	19	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	127	SER
2	H	129	LYS
3	L	152	ASN
3	L	182	SER
2	H	113	SER
3	L	211	ARG

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	179/193 (93%)	179 (100%)	0	100	100
2	H	189/189 (100%)	183 (97%)	6 (3%)	46	62
3	L	190/190 (100%)	185 (97%)	5 (3%)	54	71
All	All	558/572 (98%)	547 (98%)	11 (2%)	63	79

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	11	VAL
2	H	80	MET
2	H	82(C)	LEU
2	H	94	ARG
2	H	116	THR
2	H	215	SER
3	L	19	VAL
3	L	30	ARG
3	L	125	LEU
3	L	152	ASN
3	L	185	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1637	ASN

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Mol	Chain	Res	Type
1	A	3652	GLN
2	H	3	GLN
2	H	39	GLN
2	H	171	GLN
2	H	197	ASN
3	L	34	ASN
3	L	90	HIS
3	L	100	GLN
3	L	198	HIS
3	L	210	ASN

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	203/228 (89%)	0.40	14 (6%)	20 27	16, 25, 52, 59	0
2	H	223/223 (100%)	0.54	12 (5%)	29 38	17, 39, 58, 74	0
3	L	215/215 (100%)	0.79	20 (9%)	11 16	18, 41, 65, 71	3 (1%)
All	All	641/666 (96%)	0.58	46 (7%)	18 26	16, 36, 60, 74	3 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	214	CYS	17.6
3	L	212	GLY	12.7
3	L	153	ALA	11.8
3	L	213	GLY	10.0
3	L	154	LEU	7.5
2	H	216	CYS	7.2
3	L	155	GLN	7.1
1	A	584	GLY	5.2
3	L	184	ALA	5.1
1	A	3664	SER	4.4
1	A	3663	GLY	3.7
3	L	157	GLY	3.7
3	L	125	LEU	3.6
3	L	191	VAL	3.3
3	L	181	LEU	3.3
2	H	3	GLN	3.3
1	A	3625	HIS	3.2
3	L	150	VAL	3.1
1	A	3658	GLN	3.0
2	H	132	SER	3.0
1	A	2541	GLY	2.9
3	L	190	LYS	2.8
3	L	152	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
3	L	129	THR	2.7
3	L	210	ASN	2.6
1	A	3624	GLY	2.6
1	A	583	GLY	2.6
1	A	1664	SER	2.6
2	H	121	VAL	2.5
2	H	199	ASN	2.4
2	H	42	GLY	2.4
1	A	2578	ALA	2.4
1	A	2579	ARG	2.3
2	H	126	PRO	2.3
1	A	1626	THR	2.3
2	H	122	PHE	2.3
1	A	2581	LEU	2.2
2	H	215	SER	2.2
3	L	126	LYS	2.2
2	H	41	PRO	2.1
3	L	158	ASN	2.1
3	L	209	PHE	2.1
1	A	581	LEU	2.1
3	L	202	SER	2.1
2	H	204	ASN	2.0
2	H	205	THR	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 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.