



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:56 am GMT

PDB ID : 2H0Q
Title : Crystal Structure of the PGM domain of the Suppressor of T-Cell receptor (Sts-1)
Authors : Nassar, N.; Ford, B.; Carpino, N.
Deposited on : 2006-05-15
Resolution : 1.82 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

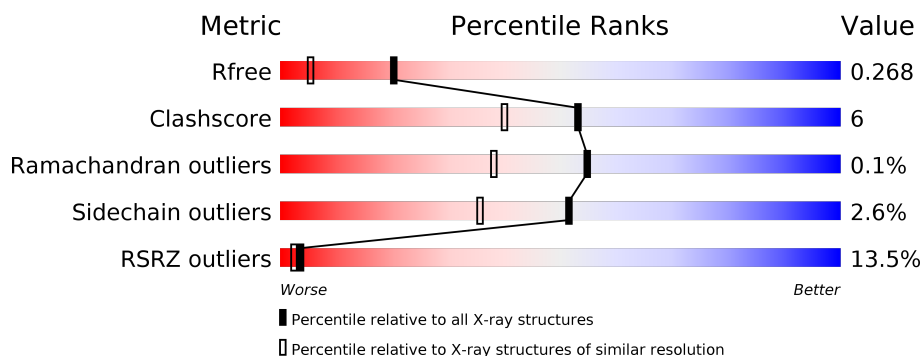
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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}	100719	5868 (1.84-1.80)
Clashscore	112137	6856 (1.84-1.80)
Ramachandran outliers	110173	6780 (1.84-1.80)
Sidechain outliers	110143	6780 (1.84-1.80)
RSRZ outliers	101464	5947 (1.84-1.80)

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	261	
1	B	261	
1	C	261	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6472 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 Suppressor of T-cell receptor signaling 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	6	0
			2066	1311	361	375	19			
1	B	256	Total	C	N	O	S	0	9	0
			2032	1287	356	372	17			
1	C	261	Total	C	N	O	S	0	2	0
			2071	1314	363	377	17			

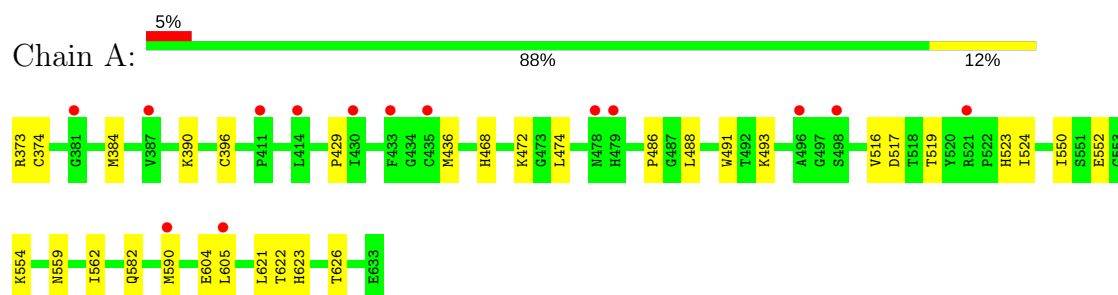
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total	O	0	0
			132	132		
2	B	109	Total	O	0	0
			109	109		
2	C	62	Total	O	0	0
			62	62		

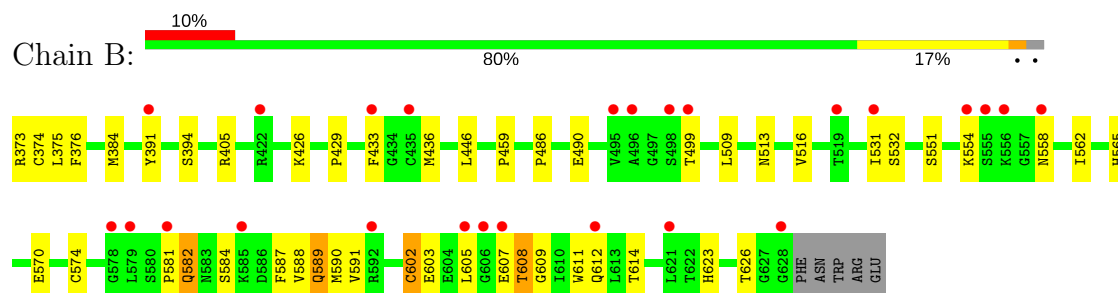
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

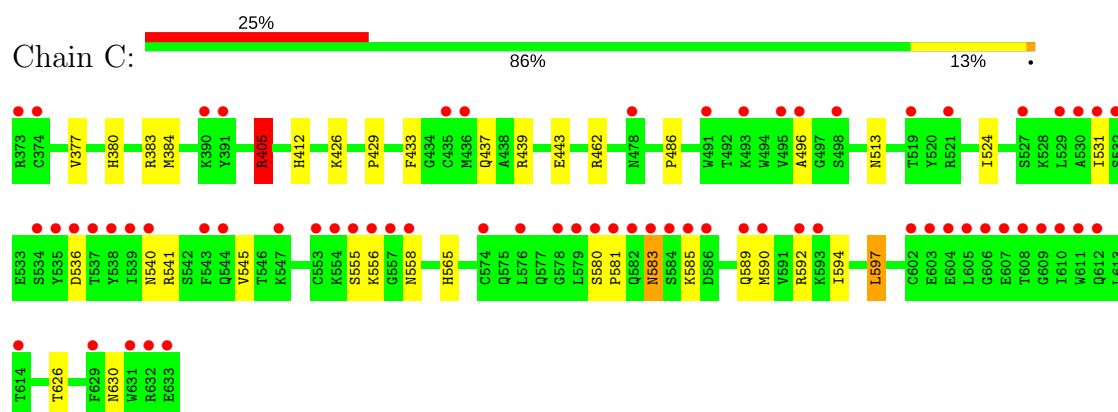
- Molecule 1: Suppressor of T-cell receptor signaling 1



- Molecule 1: Suppressor of T-cell receptor signaling 1



- Molecule 1: Suppressor of T-cell receptor signaling 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.23Å 74.34Å 100.11Å 90.00° 101.46° 90.00°	Depositor
Resolution (Å)	98.06 – 1.82 45.49 – 1.82	Depositor EDS
% Data completeness (in resolution range)	96.2 (98.06-1.82) 96.2 (45.49-1.82)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.196 , 0.236 0.232 , 0.268	Depositor DCC
R_{free} test set	3640 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6472	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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	0.67	0/2154	0.70	1/2924 (0.0%)
1	B	0.64	1/2128 (0.0%)	0.68	1/2889 (0.0%)
1	C	0.49	0/2140	0.63	2/2905 (0.1%)
All	All	0.60	1/6422 (0.0%)	0.67	4/8718 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	602	CYS	CB-SG	-6.48	1.71	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	597	LEU	CA-CB-CG	-7.45	98.17	115.30
1	B	602	CYS	CB-CA-C	-5.39	99.63	110.40
1	C	405	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	474	LEU	CA-CB-CG	5.04	126.90	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	2066	0	2038	25	0
1	B	2032	0	2023	40	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2071	0	2051	24	1
2	A	132	0	0	0	0
2	B	109	0	0	3	0
2	C	62	0	0	3	0
All	All	6472	0	6112	77	1

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 (77) 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:A:436[B]:MET:CE	1:B:436[B]:MET:HE2	1.55	1.35
1:B:570:GLU:HG2	2:B:738:HOH:O	1.36	1.22
1:A:436[B]:MET:CE	1:B:436[B]:MET:CE	2.16	1.15
1:C:462[B]:ARG:HH12	1:C:565:HIS:CE1	1.74	1.04
1:A:436[B]:MET:SD	1:B:436[B]:MET:HE3	1.67	1.02
1:A:436[B]:MET:SD	1:B:436[B]:MET:CE	0.92	0.97
1:A:622:THR:HA	1:B:626[B]:THR:HG21	1.47	0.96
1:A:436[B]:MET:SD	1:B:436[B]:MET:HE1	0.58	0.94
1:C:405:ARG:NH2	2:C:692:HOH:O	2.07	0.86
1:B:626[B]:THR:HG23	2:B:663:HOH:O	1.78	0.82
1:B:607:GLU:HG3	1:B:608:THR:N	1.98	0.76
1:A:436[B]:MET:HE3	1:B:436[B]:MET:HE2	1.65	0.75
1:A:468:HIS:NE2	1:A:472:LYS:HE3	2.05	0.72
1:C:462[B]:ARG:NH1	1:C:565:HIS:CE1	2.56	0.72
1:A:582:GLN:NE2	1:A:590[A]:MET:SD	2.64	0.70
1:A:436[B]:MET:SD	1:B:436[B]:MET:HE2	1.13	0.68
1:A:468:HIS:CD2	1:A:472:LYS:HE3	2.30	0.67
1:B:374[B]:CYS:SG	1:B:376:PHE:CE1	2.83	0.67
1:C:439:ARG:NH1	1:C:443:GLU:OE2	2.33	0.62
1:B:426:LYS:NZ	1:B:499:THR:HG23	2.16	0.59
1:C:384:MET:HG3	1:C:429:PRO:HG2	1.85	0.58
1:A:523:HIS:HE1	1:A:552:GLU:OE2	1.87	0.57
1:C:583:ASN:HD21	1:C:585:LYS:HD2	1.71	0.56
1:A:384:MET:HG3	1:A:429:PRO:HG2	1.89	0.55
1:C:462[B]:ARG:HH12	1:C:565:HIS:HE1	1.49	0.54
1:C:626:THR:HA	2:C:685:HOH:O	2.08	0.54
1:C:380:HIS:CE1	1:C:462[B]:ARG:HD2	2.45	0.51
1:B:459:PRO:HD3	1:B:486:PRO:HA	1.93	0.51
1:A:554:LYS:NZ	1:A:604:GLU:OE1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:GLU:HB2	1:B:614:THR:HG21	1.93	0.49
1:B:587:PHE:O	1:B:591:VAL:HG23	2.11	0.49
1:B:607:GLU:HG3	1:B:608:THR:H	1.74	0.48
1:C:486:PRO:HB2	1:C:524:ILE:O	2.14	0.48
1:A:491:TRP:CE2	1:A:493:LYS:HG3	2.49	0.48
1:A:621[A]:LEU:HD11	1:B:433:PHE:HE1	1.79	0.47
1:B:375:LEU:HD11	1:B:562:ILE:HD12	1.96	0.47
1:B:446:LEU:HD12	2:B:679:HOH:O	2.14	0.46
1:C:405:ARG:HD3	1:C:412:HIS:HA	1.97	0.46
1:C:555:SER:HB3	1:C:556:LYS:HG3	1.97	0.46
1:B:373:ARG:N	1:B:558:ASN:O	2.49	0.45
1:A:626:THR:HG23	1:B:623:HIS:CD2	2.52	0.45
1:B:607:GLU:O	1:B:609:GLY:N	2.44	0.45
1:C:462[A]:ARG:NH2	2:C:660:HOH:O	2.48	0.44
1:B:426:LYS:HZ2	1:B:499:THR:HG23	1.80	0.44
1:B:509:LEU:HB2	1:B:516[A]:VAL:HG21	1.97	0.44
1:C:426:LYS:NZ	1:C:496:ALA:HB3	2.32	0.44
1:B:384:MET:HG3	1:B:429:PRO:HG2	1.99	0.44
1:A:517:ASP:OD1	1:A:519:THR:HB	2.17	0.44
1:C:590:MET:CE	1:C:594:ILE:HD11	2.47	0.44
1:C:580:SER:HA	1:C:581:PRO:HD3	1.91	0.43
1:A:623:HIS:CD2	1:B:626[A]:THR:HG23	2.54	0.43
1:C:383:ARG:HG2	1:C:462[B]:ARG:HD3	2.01	0.43
1:A:486:PRO:HB2	1:A:524:ILE:O	2.19	0.43
1:B:490:GLU:HB3	1:B:565:HIS:CG	2.54	0.43
1:B:582:GLN:NE2	1:B:590[B]:MET:SD	2.91	0.42
1:A:374:CYS:HB2	1:A:559:ASN:OD1	2.18	0.42
1:C:433:PHE:O	1:C:437:GLN:HG3	2.19	0.42
1:C:462[B]:ARG:HH12	1:C:565:HIS:HD1	1.60	0.42
1:B:605:LEU:HD21	1:B:612:GLN:NE2	2.34	0.42
1:C:541:ARG:O	1:C:545:VAL:HG23	2.19	0.42
1:B:426:LYS:NZ	1:B:499:THR:CG2	2.83	0.42
1:A:488:LEU:HD13	1:A:562:ILE:HG23	2.02	0.41
1:B:374[B]:CYS:SG	1:B:376:PHE:CZ	3.10	0.41
1:B:551:SER:HA	1:B:554:LYS:HG3	2.02	0.41
1:C:536:ASP:O	1:C:540:ASN:ND2	2.54	0.41
1:A:468:HIS:HE2	1:A:472:LYS:HE3	1.82	0.41
1:A:550:ILE:O	1:A:554:LYS:HG2	2.20	0.41
1:C:589:GLN:HG3	1:C:592:ARG:NH1	2.35	0.41
1:C:462[B]:ARG:NH1	1:C:565:HIS:ND1	2.60	0.41
1:B:574:CYS:SG	1:B:581:PRO:HA	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:CYS:HB3	1:B:611:TRP:HB3	2.03	0.41
1:B:513:ASN:HB2	1:C:513:ASN:CG	2.41	0.40
1:B:607:GLU:C	1:B:609:GLY:H	2.25	0.40
1:B:584:SER:O	1:B:588:VAL:HG23	2.21	0.40

All (1) 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)
1:B:391:TYR:OH	1:C:540:ASN:ND2[3_555]	2.16	0.04

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	265/261 (102%)	259 (98%)	6 (2%)	0	100	100
1	B	263/261 (101%)	252 (96%)	10 (4%)	1 (0%)	38	22
1	C	262/261 (100%)	252 (96%)	10 (4%)	0	100	100
All	All	790/783 (101%)	763 (97%)	26 (3%)	1 (0%)	55	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	608	THR

5.3.2 Protein sidechains [i](#)

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	234/229 (102%)	228 (97%)	6 (3%)	51	36
1	B	233/229 (102%)	226 (97%)	7 (3%)	46	29
1	C	232/229 (101%)	225 (97%)	7 (3%)	46	29
All	All	699/687 (102%)	679 (97%)	20 (3%)	51	31

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	ARG
1	A	390	LYS
1	A	396[A]	CYS
1	A	396[B]	CYS
1	A	516	VAL
1	A	605	LEU
1	B	394	SER
1	B	405[A]	ARG
1	B	405[B]	ARG
1	B	531	ILE
1	B	532	SER
1	B	582	GLN
1	B	589	GLN
1	C	377	VAL
1	C	405	ARG
1	C	531	ILE
1	C	558	ASN
1	C	583	ASN
1	C	597	LEU
1	C	630	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	523	HIS
1	B	412	HIS
1	B	577	GLN
1	B	582	GLN
1	B	612	GLN
1	C	412	HIS

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Mol	Chain	Res	Type
1	C	558	ASN
1	C	630	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	261/261 (100%)	0.48	14 (5%) 26 22	20, 30, 43, 50	0
1	B	256/261 (98%)	0.68	25 (9%) 8 6	23, 31, 45, 51	0
1	C	261/261 (100%)	1.19	66 (25%) 1 0	26, 38, 49, 55	0
All	All	778/783 (99%)	0.78	105 (13%) 3 2	20, 33, 46, 55	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	ALA	9.4
1	C	605	LEU	7.7
1	C	610	ILE	7.0
1	C	531	ILE	6.7
1	C	606	GLY	5.9
1	C	555	SER	5.8
1	C	496	ALA	5.6
1	C	537	THR	5.5
1	C	578	GLY	5.5
1	C	579	LEU	5.3
1	C	631	TRP	5.1
1	C	543	PHE	4.9
1	C	536	ASP	4.9
1	B	628	GLY	4.8
1	A	605	LEU	4.8
1	C	607	GLU	4.7
1	B	605	LEU	4.3
1	B	555	SER	4.2
1	C	530	ALA	4.2
1	C	498	SER	4.2
1	C	556	LYS	4.1
1	B	531	ILE	4.1
1	A	498	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	632	ARG	4.0
1	C	611	TRP	4.0
1	C	576	LEU	4.0
1	A	478	ASN	3.8
1	B	498	SER	3.8
1	C	608	THR	3.7
1	C	491	TRP	3.7
1	C	534	SER	3.7
1	C	521	ARG	3.6
1	A	479	HIS	3.6
1	B	606	GLY	3.5
1	C	585	LYS	3.5
1	C	558	ASN	3.5
1	C	557	GLY	3.4
1	C	602	CYS	3.3
1	C	478	ASN	3.2
1	C	373	ARG	3.2
1	B	499	THR	3.2
1	C	538	TYR	3.2
1	C	580	SER	3.2
1	B	607	GLU	3.1
1	B	391	TYR	3.1
1	B	579	LEU	3.0
1	C	554	LYS	3.0
1	C	590	MET	3.0
1	C	609	GLY	3.0
1	C	495	VAL	3.0
1	C	540	ASN	2.9
1	C	527	SER	2.9
1	C	584	SER	2.9
1	C	391	TYR	2.9
1	B	435	CYS	2.9
1	B	578	GLY	2.8
1	C	535	TYR	2.8
1	B	581	PRO	2.7
1	C	581	PRO	2.7
1	C	539	ILE	2.7
1	C	574	CYS	2.7
1	B	556	LYS	2.7
1	C	553	CYS	2.6
1	B	433	PHE	2.6
1	A	496	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	603	GLU	2.6
1	C	586	ASP	2.6
1	A	433	PHE	2.5
1	B	585	LYS	2.5
1	C	547	LYS	2.5
1	A	381	GLY	2.5
1	C	435	CYS	2.5
1	B	554	LYS	2.5
1	A	435	CYS	2.5
1	C	592	ARG	2.5
1	C	612	GLN	2.4
1	C	582	GLN	2.4
1	A	387	VAL	2.4
1	C	493	LYS	2.4
1	C	519	THR	2.4
1	C	614	THR	2.4
1	C	604	GLU	2.4
1	A	590[A]	MET	2.3
1	C	529	LEU	2.3
1	B	592	ARG	2.3
1	B	495	VAL	2.3
1	B	612	GLN	2.3
1	C	589	GLN	2.2
1	A	414	LEU	2.2
1	B	422	ARG	2.2
1	C	532	SER	2.2
1	C	544	GLN	2.2
1	A	411	PRO	2.2
1	B	558	ASN	2.1
1	C	633	GLU	2.1
1	B	621	LEU	2.1
1	C	374	CYS	2.1
1	A	521	ARG	2.0
1	B	519[A]	THR	2.0
1	C	436[A]	MET	2.0
1	C	593	LYS	2.0
1	C	629	PHE	2.0
1	A	430	ILE	2.0
1	C	583	ASN	2.0
1	C	390	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 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.