



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 7, 2024 – 12:06 pm GMT

PDB ID : 8RD2
Title : Trypanosoma brucei Invariant Surface Glycoprotein 75 (ISG75)
Authors : Stodkilde-Jorgensen, K.; Mikkelsen, J.H.
Deposited on : 2023-12-07
Resolution : 2.69 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

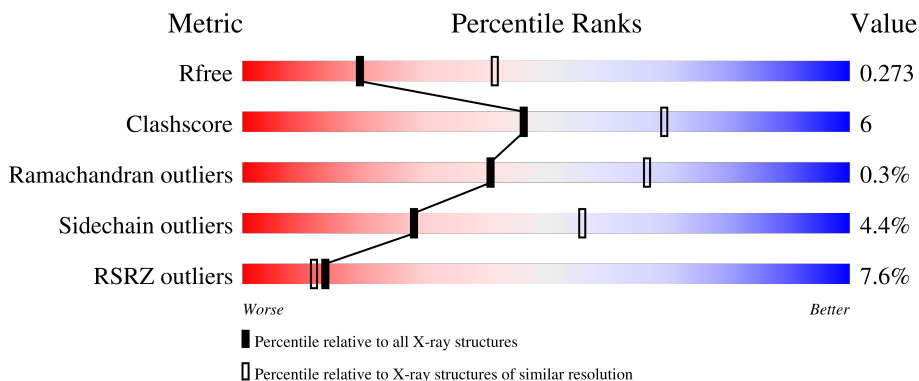
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	440	 5% 75% 14% • 10%
1	B	440	 9% 72% 18% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6261 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 Invariant surface glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	398	3121	1921	562	622	16	0	0	0
1	B	400	3140	1933	567	624	16	0	0	0

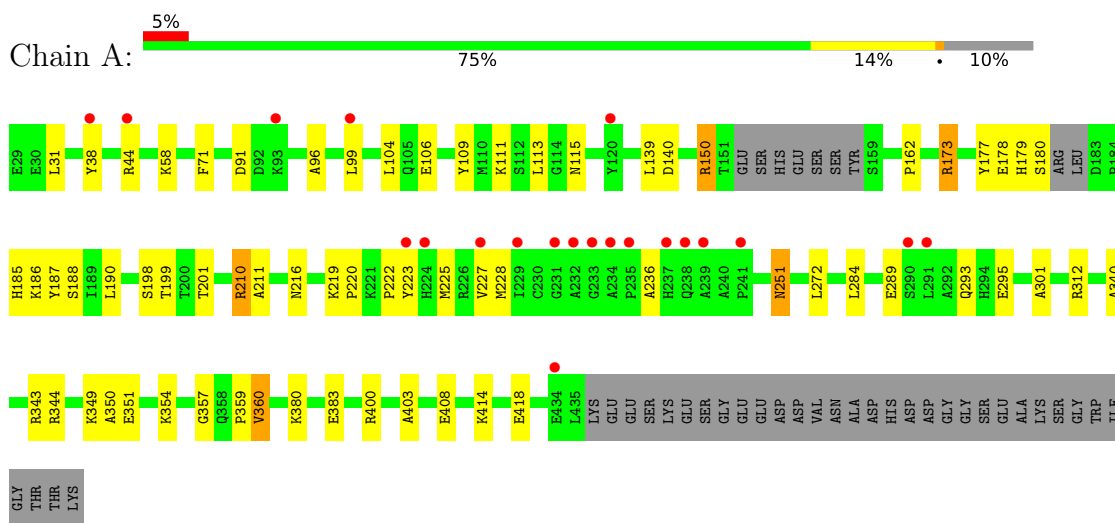
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	ALA	ASN	engineered mutation	UNP Q26769
B	134	ALA	ASN	engineered mutation	UNP Q26769

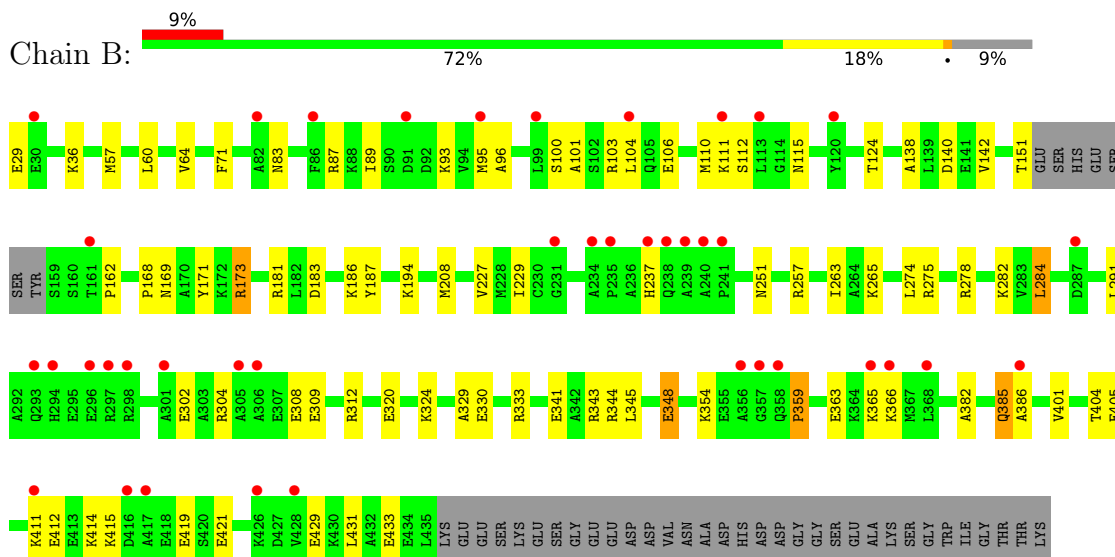
3 Residue-property plots i

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: Invariant surface glycoprotein



- Molecule 1: Invariant surface glycoprotein



4 Data and refinement statistics i

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	120.01Å 120.01Å 107.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.67 – 2.69 53.67 – 2.69	Depositor EDS
% Data completeness (in resolution range)	52.0 (53.67-2.69) 52.0 (53.67-2.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.228 , 0.272 0.233 , 0.273	Depositor DCC
R_{free} test set	1223 reflections (5.53%)	wwPDB-VP
Wilson B-factor (Å ²)	82.7	Xtrriage
Anisotropy	0.034	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.041 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6261	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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	0.24	0/3160	0.46	0/4240
1	B	0.24	0/3180	0.45	0/4268
All	All	0.24	0/6340	0.45	0/8508

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	3121	0	3094	35	0
1	B	3140	0	3119	45	0
All	All	6261	0	6213	79	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 (79) 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:173:ARG:NH1	1:B:183:ASP:OD2	2.17	0.77
1:A:44:ARG:HD3	1:A:220:PRO:HA	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLU:HB3	1:A:293:GLN:H	1.55	0.71
1:A:216:ASN:HA	1:A:219:LYS:HD2	1.72	0.70
1:A:111:LYS:O	1:A:115:ASN:ND2	2.28	0.66
1:B:181:ARG:HH11	1:B:344:ARG:HH12	1.44	0.63
1:A:414:LYS:NZ	1:A:418:GLU:OE2	2.30	0.61
1:B:173:ARG:HH12	1:B:186:LYS:HA	1.67	0.59
1:A:96:ALA:HA	1:A:99:LEU:HD12	1.86	0.57
1:B:36:LYS:HD3	1:B:229:ILE:HD13	1.86	0.56
1:A:113:LEU:HD21	1:A:272:LEU:HD11	1.86	0.56
1:A:223:TYR:CZ	1:A:225:MET:HB2	2.41	0.55
1:A:350:ALA:HB1	1:A:360:VAL:HG21	1.89	0.55
1:B:302:GLU:HG2	1:B:414:LYS:HE3	1.90	0.54
1:B:60:LEU:HD13	1:B:208:MET:HA	1.90	0.53
1:B:57:MET:HA	1:B:60:LEU:HD12	1.90	0.53
1:A:251:ASN:OD1	1:A:251:ASN:N	2.34	0.52
1:B:345:LEU:HA	1:B:348:GLU:HB2	1.92	0.52
1:B:312:ARG:HD2	1:B:404:THR:HG23	1.91	0.52
1:B:429:GLU:O	1:B:433:GLU:HG2	2.10	0.52
1:B:308:GLU:O	1:B:312:ARG:N	2.43	0.51
1:A:312:ARG:HA	1:A:403:ALA:HB1	1.93	0.50
1:B:282:LYS:HB3	1:B:421:GLU:HG3	1.93	0.50
1:B:309:GLU:OE2	1:B:411:LYS:NZ	2.45	0.50
1:A:91:ASP:HB3	1:B:366:LYS:NZ	2.26	0.50
1:B:415:LYS:O	1:B:419:GLU:HG2	2.11	0.49
1:B:320:GLU:OE2	1:B:324:LYS:HE2	2.12	0.49
1:A:177:TYR:CD2	1:A:180:SER:HB3	2.48	0.48
1:A:351:GLU:OE2	1:A:354:LYS:HD3	2.13	0.48
1:A:186:LYS:HG2	1:A:187:TYR:H	1.79	0.48
1:A:106:GLU:HA	1:A:109:TYR:HB3	1.94	0.48
1:A:178:GLU:O	1:A:179:HIS:HB3	2.13	0.48
1:B:274:LEU:HD21	1:B:412:GLU:OE2	2.14	0.47
1:A:99:LEU:HD13	1:A:104:LEU:HD12	1.96	0.47
1:B:329:ALA:HB1	1:B:386:ALA:HA	1.98	0.46
1:B:274:LEU:HD11	1:B:278:ARG:HE	1.80	0.46
1:A:210:ARG:HG3	1:A:211:ALA:N	2.30	0.46
1:B:124:THR:HG21	1:B:265:LYS:HD3	1.98	0.46
1:A:380:LYS:HA	1:A:383:GLU:OE2	2.16	0.45
1:B:89:ILE:HG23	1:B:95:MET:HG3	1.98	0.45
1:A:349:LYS:HD3	1:A:349:LYS:HA	1.79	0.45
1:A:301:ALA:HB1	1:A:414:LYS:HA	1.97	0.45
1:B:111:LYS:HE3	1:B:115:ASN:HD21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ARG:NH2	1:A:188:SER:O	2.49	0.45
1:B:341:GLU:HA	1:B:344:ARG:HD2	1.98	0.45
1:B:168:PRO:HA	1:B:171:TYR:CZ	2.52	0.45
1:B:169:ASN:O	1:B:194:LYS:NZ	2.29	0.44
1:B:365:LYS:HA	1:B:365:LYS:HD2	1.72	0.44
1:A:31:LEU:HG	1:A:38:TYR:CZ	2.52	0.44
1:B:251:ASN:OD1	1:B:251:ASN:N	2.51	0.44
1:B:64:VAL:HG13	1:B:263:ILE:HD11	1.99	0.44
1:B:89:ILE:HD11	1:B:284:LEU:HA	2.00	0.43
1:B:83:ASN:O	1:B:87:ARG:HG3	2.18	0.43
1:A:179:HIS:CG	1:A:179:HIS:O	2.71	0.43
1:B:274:LEU:O	1:B:278:ARG:HG2	2.18	0.43
1:A:31:LEU:HD11	1:A:227:VAL:HG13	2.00	0.43
1:A:357:GLY:O	1:A:359:PRO:HD3	2.19	0.43
1:B:304:ARG:O	1:B:308:GLU:HG2	2.19	0.43
1:B:401:VAL:O	1:B:405:GLU:HG2	2.19	0.42
1:A:162:PRO:HD3	1:A:187:TYR:CZ	2.55	0.42
1:A:199:THR:HA	1:A:400:ARG:HH22	1.85	0.42
1:B:138:ALA:O	1:B:142:VAL:HG23	2.20	0.42
1:A:340:ALA:O	1:A:344:ARG:HG2	2.20	0.42
1:B:330:GLU:OE1	1:B:333:ARG:NE	2.49	0.41
1:A:198:SER:N	1:A:201:THR:OG1	2.50	0.41
1:B:29:GLU:HG3	1:B:227:VAL:HG21	2.03	0.41
1:B:93:LYS:HA	1:B:96:ALA:HB3	2.03	0.41
1:B:382:ALA:HA	1:B:385:GLN:HB2	2.02	0.41
1:B:100:SER:HB2	1:B:103:ARG:HB3	2.03	0.41
1:B:275:ARG:HA	1:B:275:ARG:HD3	1.89	0.41
1:A:162:PRO:HB3	1:A:187:TYR:CD1	2.56	0.41
1:B:101:ALA:O	1:B:104:LEU:HB3	2.21	0.41
1:B:162:PRO:HD3	1:B:187:TYR:CZ	2.55	0.41
1:A:150:ARG:HE	1:A:150:ARG:HB3	1.64	0.40
1:B:354:LYS:HA	1:B:359:PRO:O	2.22	0.40
1:A:38:TYR:HB2	1:A:222:PRO:HB3	2.02	0.40
1:A:58:LYS:HB2	1:A:139:LEU:HD23	2.03	0.40
1:B:111:LYS:HE2	1:B:111:LYS:HB3	1.78	0.40
1:B:106:GLU:O	1:B:110:MET:HG2	2.20	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	392/440 (89%)	373 (95%)	18 (5%)	1 (0%)	41	66
1	B	396/440 (90%)	379 (96%)	16 (4%)	1 (0%)	41	66
All	All	788/880 (90%)	752 (95%)	34 (4%)	2 (0%)	41	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	359	PRO
1	A	236	ALA

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	319/354 (90%)	305 (96%)	14 (4%)	28	56
1	B	321/354 (91%)	307 (96%)	14 (4%)	28	56
All	All	640/708 (90%)	612 (96%)	28 (4%)	28	56

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	PHE
1	A	140	ASP
1	A	150	ARG
1	A	173	ARG

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Mol	Chain	Res	Type
1	A	185	HIS
1	A	190	LEU
1	A	210	ARG
1	A	228	MET
1	A	251	ASN
1	A	284	LEU
1	A	295	GLU
1	A	343	ARG
1	A	360	VAL
1	A	408	GLU
1	B	71	PHE
1	B	112	SER
1	B	140	ASP
1	B	151	THR
1	B	173	ARG
1	B	237	HIS
1	B	257	ARG
1	B	284	LEU
1	B	291	LEU
1	B	343	ARG
1	B	348	GLU
1	B	363	GLU
1	B	385	GLN
1	B	431	LEU

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	238	GLN
1	B	45	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 monosaccharides 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	398/440 (90%)	0.58	21 (5%) 26 25	35, 77, 160, 236	0
1	B	400/440 (90%)	0.76	40 (10%) 7 5	39, 94, 165, 205	0
All	All	798/880 (90%)	0.67	61 (7%) 13 12	35, 86, 162, 236	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	357	GLY	7.6
1	A	232	ALA	6.6
1	A	290	SER	6.5
1	B	120	TYR	5.4
1	B	293	GLN	5.1
1	B	297	ARG	4.9
1	B	237	HIS	4.8
1	B	113	LEU	4.8
1	B	411	LYS	4.6
1	B	239	ALA	3.9
1	A	44	ARG	3.7
1	B	240	ALA	3.6
1	B	368	LEU	3.5
1	A	241	PRO	3.5
1	A	234	ALA	3.4
1	B	356	ALA	3.4
1	A	233	GLY	3.3
1	A	227	VAL	3.2
1	B	365	LYS	3.2
1	A	238	GLN	3.2
1	B	82	ALA	3.1
1	A	235	PRO	3.1
1	B	86	PHE	3.1
1	B	298	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	239	ALA	3.0
1	B	95	MET	3.0
1	A	229	ILE	2.9
1	B	366	LYS	2.9
1	B	99	LEU	2.8
1	B	417	ALA	2.8
1	B	111	LYS	2.8
1	A	231	GLY	2.8
1	B	235	PRO	2.7
1	B	287	ASP	2.7
1	B	241	PRO	2.6
1	A	237	HIS	2.6
1	B	426	LYS	2.6
1	B	358	GLN	2.6
1	A	224	HIS	2.6
1	A	99	LEU	2.6
1	B	416	ASP	2.6
1	B	305	ALA	2.5
1	B	104	LEU	2.5
1	B	428	VAL	2.4
1	B	91	ASP	2.4
1	B	386	ALA	2.3
1	B	301	ALA	2.3
1	A	223	TYR	2.3
1	A	93	LYS	2.3
1	A	38	TYR	2.3
1	A	434	GLU	2.2
1	B	238	GLN	2.2
1	B	234	ALA	2.1
1	B	296	GLU	2.1
1	A	291	LEU	2.1
1	B	161	THR	2.1
1	B	231	GLY	2.1
1	B	306	ALA	2.1
1	B	30	GLU	2.1
1	A	120	TYR	2.0
1	B	294	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.