



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:10 am BST

PDB ID : 4JHR
Title : An auto-inhibited conformation of LGN reveals a distinct interaction mode between GoLoco motifs and TPR motifs
Authors : Pan, Z.; Zhu, J.; Shang, Y.; Wei, Z.; Jia, M.; Xia, C.; Wen, W.; Wang, W.; Zhang, M.
Deposited on : 2013-03-05
Resolution : 2.80 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 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 : 2.11
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) : 2.11

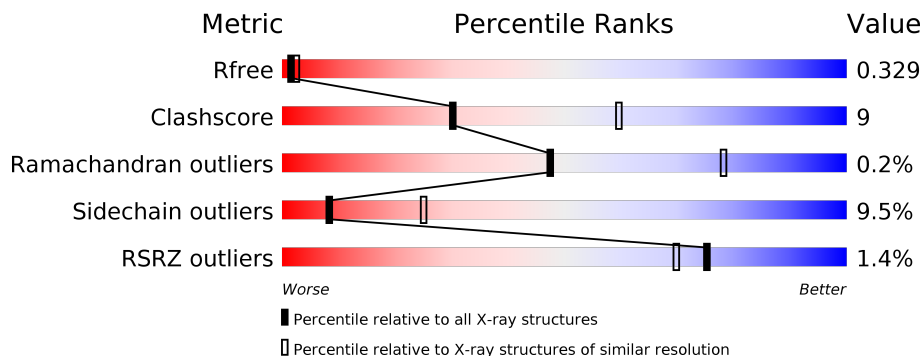
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	333	 2% 66% 17% 13%
1	B	333	 69% 14% 13%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 4249 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 G-protein-signaling modulator 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	290	Total	C	N	O	S	0	0	0
			2148	1342	378	421	7			
1	B	289	Total	C	N	O	S	0	0	0
			2101	1315	373	407	6			

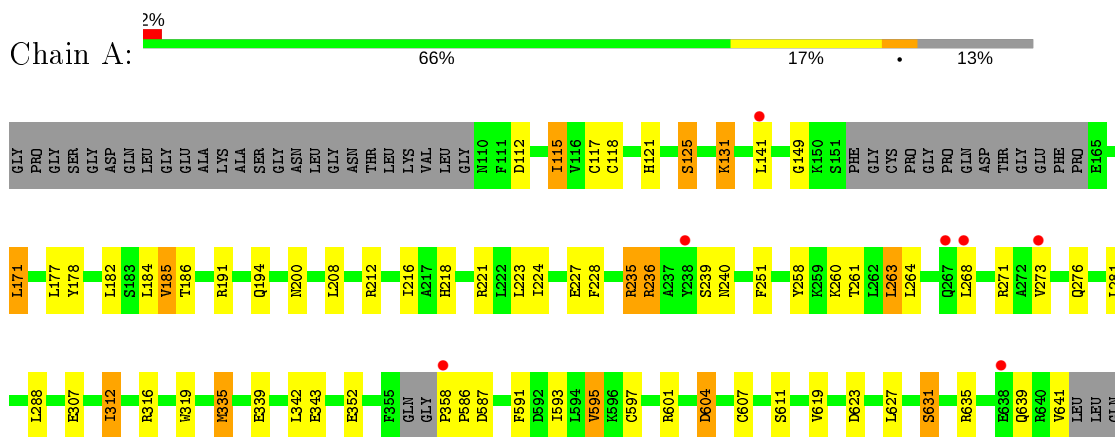
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	GLY	-	EXPRESSION TAG	UNP Q8VDU0
A	86	PRO	-	EXPRESSION TAG	UNP Q8VDU0
A	87	GLY	-	EXPRESSION TAG	UNP Q8VDU0
A	88	SER	-	EXPRESSION TAG	UNP Q8VDU0
A	351	LEU	-	EXPRESSION TAG	UNP Q8VDU0
A	352	GLU	-	EXPRESSION TAG	UNP Q8VDU0
A	353	VAL	-	EXPRESSION TAG	UNP Q8VDU0
A	354	LEU	-	EXPRESSION TAG	UNP Q8VDU0
A	355	PHE	-	EXPRESSION TAG	UNP Q8VDU0
A	356	GLN	-	EXPRESSION TAG	UNP Q8VDU0
A	357	GLY	-	EXPRESSION TAG	UNP Q8VDU0
A	358	PRO	-	EXPRESSION TAG	UNP Q8VDU0
B	85	GLY	-	EXPRESSION TAG	UNP Q8VDU0
B	86	PRO	-	EXPRESSION TAG	UNP Q8VDU0
B	87	GLY	-	EXPRESSION TAG	UNP Q8VDU0
B	88	SER	-	EXPRESSION TAG	UNP Q8VDU0
B	351	LEU	-	EXPRESSION TAG	UNP Q8VDU0
B	352	GLU	-	EXPRESSION TAG	UNP Q8VDU0
B	353	VAL	-	EXPRESSION TAG	UNP Q8VDU0
B	354	LEU	-	EXPRESSION TAG	UNP Q8VDU0
B	355	PHE	-	EXPRESSION TAG	UNP Q8VDU0
B	356	GLN	-	EXPRESSION TAG	UNP Q8VDU0
B	357	GLY	-	EXPRESSION TAG	UNP Q8VDU0
B	358	PRO	-	EXPRESSION TAG	UNP Q8VDU0

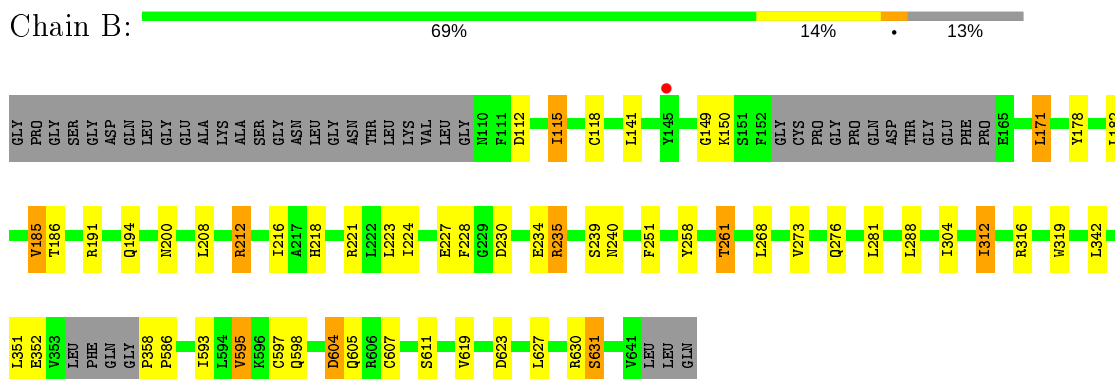
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: G-protein-signaling modulator 2



- Molecule 1: G-protein-signaling modulator 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.21Å 81.80Å 106.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.04 – 2.80 38.04 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.2 (38.04-2.80) 99.7 (38.04-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.250 , 0.311 0.266 , 0.329	Depositor DCC
R_{free} test set	817 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtrriage
Anisotropy	0.836	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4249	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3928e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.43	0/2185	0.67	3/2972 (0.1%)
1	B	0.42	0/2138	0.67	3/2913 (0.1%)
All	All	0.43	0/4323	0.67	6/5885 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ARG	NE-CZ-NH2	12.52	126.56	120.30
1	A	221	ARG	NE-CZ-NH1	-12.36	114.12	120.30
1	B	221	ARG	NE-CZ-NH2	-12.07	114.26	120.30
1	B	221	ARG	NE-CZ-NH1	11.59	126.09	120.30
1	A	221	ARG	CD-NE-CZ	6.74	133.04	123.60
1	B	221	ARG	CD-NE-CZ	5.71	131.59	123.60

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	2148	0	1938	42	0
1	B	2101	0	1872	35	0
All	All	4249	0	3810	75	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 9.

All (75) 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:149:GLY:HA3	1:A:171:LEU:HD13	1.59	0.83
1:B:149:GLY:HA3	1:B:171:LEU:HD13	1.65	0.79
1:A:186:THR:HA	1:A:194:GLN:HE21	1.50	0.74
1:A:235:ARG:HD2	1:A:273:VAL:HG11	1.70	0.74
1:B:186:THR:HA	1:B:194:GLN:HE21	1.52	0.73
1:B:235:ARG:HD2	1:B:273:VAL:HG11	1.69	0.73
1:A:271:ARG:NE	1:A:307:GLU:OE1	2.20	0.71
1:B:118:CYS:HB2	1:B:141:LEU:HD13	1.72	0.69
1:B:171:LEU:HB3	1:B:208:LEU:HD21	1.74	0.69
1:B:185:VAL:HG12	1:B:194:GLN:HG3	1.74	0.68
1:A:185:VAL:HG12	1:A:194:GLN:HG3	1.74	0.68
1:A:118:CYS:HB2	1:A:141:LEU:HD13	1.75	0.68
1:A:260:LYS:HA	1:A:263:LEU:HD23	1.76	0.67
1:B:604:ASP:OD2	1:B:604:ASP:N	2.33	0.62
1:A:604:ASP:OD2	1:A:604:ASP:N	2.33	0.61
1:A:352:GLU:O	1:A:611:SER:OG	2.18	0.59
1:A:235:ARG:HH22	1:A:236:ARG:HH11	1.52	0.58
1:A:251:PHE:HB2	1:A:288:LEU:HD21	1.84	0.58
1:A:258:TYR:O	1:A:261:THR:HG22	2.04	0.57
1:A:635:ARG:O	1:A:639:GLN:HG2	2.04	0.57
1:B:352:GLU:O	1:B:611:SER:OG	2.22	0.57
1:A:171:LEU:HB3	1:A:208:LEU:HD21	1.87	0.56
1:B:251:PHE:HB2	1:B:288:LEU:HD21	1.87	0.54
1:A:335:MET:O	1:A:339:GLU:HG2	2.08	0.54
1:B:178:TYR:CE2	1:B:200:ASN:HB3	2.42	0.54
1:A:186:THR:HA	1:A:194:GLN:NE2	2.22	0.54
1:A:319:TRP:CE2	1:A:595:VAL:HG22	2.43	0.53
1:A:235:ARG:HG2	1:A:261:THR:OG1	2.09	0.53
1:B:258:TYR:O	1:B:261:THR:HG22	2.09	0.53
1:B:186:THR:HA	1:B:194:GLN:NE2	2.24	0.52
1:B:316:ARG:NH1	1:B:623:ASP:OD1	2.41	0.52
1:A:224:ILE:O	1:A:228:PHE:HD2	1.92	0.52
1:A:223:LEU:O	1:A:227:GLU:HG3	2.10	0.51
1:B:224:ILE:O	1:B:228:PHE:HD2	1.94	0.51
1:B:182:LEU:O	1:B:186:THR:OG1	2.24	0.50
1:A:212:ARG:O	1:A:216:ILE:HD12	2.12	0.50
1:A:112:ASP:HA	1:A:115:ILE:HG22	1.92	0.50
1:B:112:ASP:HA	1:B:115:ILE:HG22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLU:O	1:A:343:GLU:HG3	2.13	0.48
1:A:235:ARG:CD	1:A:273:VAL:HG11	2.43	0.48
1:B:258:TYR:HB3	1:B:281:LEU:HG	1.96	0.47
1:A:258:TYR:HB3	1:A:281:LEU:HG	1.96	0.47
1:A:178:TYR:CE2	1:A:200:ASN:HB3	2.49	0.47
1:B:223:LEU:O	1:B:227:GLU:HG3	2.14	0.47
1:B:319:TRP:CE2	1:B:595:VAL:HG22	2.49	0.47
1:A:182:LEU:O	1:A:186:THR:OG1	2.25	0.46
1:A:276:GLN:NE2	1:A:619:VAL:O	2.38	0.46
1:B:593:ILE:HD11	1:B:607:CYS:HB2	1.98	0.46
1:B:235:ARG:HG2	1:B:261:THR:OG1	2.15	0.46
1:B:230:ASP:O	1:B:234:GLU:HB2	2.16	0.45
1:A:131:LYS:HE2	1:A:184:LEU:HD11	1.98	0.45
1:B:191:ARG:HD2	1:B:194:GLN:OE1	2.18	0.44
1:B:212:ARG:O	1:B:216:ILE:HD12	2.18	0.44
1:B:630:ARG:HD3	1:B:630:ARG:HA	1.64	0.44
1:A:121:HIS:O	1:A:125:SER:OG	2.32	0.43
1:A:191:ARG:HD2	1:A:194:GLN:OE1	2.18	0.43
1:A:358:PRO:HA	1:A:586:PRO:HD3	1.84	0.43
1:A:627:LEU:O	1:A:631:SER:HB3	2.17	0.43
1:B:312:ILE:HG12	1:B:312:ILE:H	1.64	0.43
1:A:218:HIS:CE1	1:A:240:ASN:HB3	2.53	0.43
1:A:586:PRO:HG3	1:B:586:PRO:HG3	2.01	0.43
1:B:171:LEU:HA	1:B:171:LEU:HD12	1.75	0.43
1:A:264:LEU:HA	1:A:264:LEU:HD23	1.84	0.43
1:B:627:LEU:O	1:B:631:SER:HB3	2.18	0.42
1:A:591:PHE:O	1:A:595:VAL:HB	2.19	0.42
1:B:288:LEU:HA	1:B:288:LEU:HD23	1.80	0.42
1:A:117:CYS:HB3	1:B:605:GLN:HE22	1.85	0.42
1:B:276:GLN:NE2	1:B:619:VAL:O	2.45	0.42
1:A:312:ILE:H	1:A:312:ILE:HG12	1.67	0.41
1:B:218:HIS:CE1	1:B:240:ASN:HB3	2.55	0.41
1:B:358:PRO:HA	1:B:586:PRO:HD3	1.84	0.41
1:B:235:ARG:CD	1:B:273:VAL:HG11	2.44	0.41
1:A:593:ILE:HD11	1:A:607:CYS:HB2	2.03	0.40
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.91	0.40
1:A:316:ARG:NH1	1:A:623:ASP:OD1	2.54	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	284/333 (85%)	276 (97%)	7 (2%)	1 (0%)	34	66
1	B	283/333 (85%)	273 (96%)	10 (4%)	0	100	100
All	All	567/666 (85%)	549 (97%)	17 (3%)	1 (0%)	47	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	587	ASP

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	201/267 (75%)	182 (90%)	19 (10%)	8	25
1	B	190/267 (71%)	172 (90%)	18 (10%)	8	25
All	All	391/534 (73%)	354 (90%)	37 (10%)	8	25

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ILE
1	A	125	SER
1	A	131	LYS
1	A	171	LEU
1	A	185	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	235	ARG
1	A	236	ARG
1	A	239	SER
1	A	263	LEU
1	A	268	LEU
1	A	312	ILE
1	A	335	MET
1	A	342	LEU
1	A	595	VAL
1	A	597	CYS
1	A	601	ARG
1	A	604	ASP
1	A	631	SER
1	A	641	VAL
1	B	115	ILE
1	B	150	LYS
1	B	171	LEU
1	B	185	VAL
1	B	212	ARG
1	B	235	ARG
1	B	239	SER
1	B	261	THR
1	B	268	LEU
1	B	304	ILE
1	B	312	ILE
1	B	342	LEU
1	B	351	LEU
1	B	595	VAL
1	B	597	CYS
1	B	598	GLN
1	B	604	ASP
1	B	631	SER

Some 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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	290/333 (87%)	0.01	7 (2%) 59 49	57, 75, 95, 105	0
1	B	289/333 (86%)	0.03	1 (0%) 94 93	54, 73, 94, 108	0
All	All	579/666 (86%)	0.02	8 (1%) 75 70	54, 74, 95, 108	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	VAL	2.5
1	A	268	LEU	2.5
1	A	638	GLU	2.5
1	A	358	PRO	2.4
1	A	141	LEU	2.3
1	A	238	TYR	2.3
1	A	267	GLN	2.2
1	B	145	TYR	2.2

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.